

Faculty of Natural Sciences

University of Ss. Cyril and Methodius in Trnava

The 8th International Scientific Conference
Applied Natural Sciences 2023



ANS 2023

Book of abstracts



UNIVERZITA J. E. PURKYNĚ V ÚSTÍ NAD LABEM



18th – 20th of September 2023
Donovaly, Slovakia

University of Ss. Cyril and Methodius in Trnava

Faculty of Natural Sciences

Applied Natural Sciences 2023 – Book of Abstracts

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1. Chemistry and Environmental Science
2. Biology and Biotechnology
3. Applied Informatics
4. Young Scientists

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The publication has passed the review process.

ISBN 978-80-572-0357-5

FOREWORD

Dear ladies and gentlemen,

It is my great honour to welcome you at the 8th International Scientific Conference „Applied Natural Sciences 2023“, ANS 2023, organized by our Faculty of Natural Sciences, University of Ss. Cyril and Methodius in Trnava in cooperation with the University of Jan Evangelista Purkyně in Ústí nad Labem, Czech Republic.

The ANS 2023 Conference embraces multiple challenges with a programme that offers plentiful opportunities for debate and discussion. We are proud that this conference was again organized with a constant encouragement and the support from several scientific journals, including the International Journal of Environmental Sciences and Technology, Nova Biotechnologica et Chimica and Journal of Applied Mathematics, Statistics and Informatics and journal Biologia. We are therefore delighted to provide a brilliant platform for you, the researchers to share and explore your knowledge, and consequently to publish and present your research work in these journals and present your research reports in this annual conclave. I am glad that you, renowned lecturers, have made your way to the Donovaly, the picturesque part of Slovakia. I would like to thank you for willing to present highlights and latest research findings during these conference days and thus for giving all participants the opportunity to benefit from contribution to knowledge.

I am delighted that, after the hiatus caused by the COVID 19 pandemic, we are continuing in the fine tradition of previous conferences in this ANS 2023 series. Designed to attract an international community of scientists who wish to share their interests in the broad and exciting areas of the life sciences, including chemistry and biomedical chemistry, biology and molecular biology, biotechnology and environmental technology, as well as applied informatics, the ANS 2023 conference will be a great success story for the ANS 2023 community. It is gratifying that the conference has a broad cross-curricular dimension and interdisciplinarity. We are very pleased to welcome around 100 participants, where a large number of participants are renowned colleagues from both academia and industry. We are also pleased that the majority of the participants are young researchers, postdoctoral fellows and PhD students who will present their latest research results at the Young Scientists Symposium. The conference programme aims to document the high level of scientific research at the participating universities, as well as to acknowledge the experience of our colleagues from Slovakia and abroad who will be attending the conference. The conference is also a platform for young scientists and PhD students to present and discuss their results. I would like to express my sincere gratitude and appreciation to all the speakers, not only from abroad. Last but not least, I would especially like to thank the team of people from the organizing committee.

I am very pleased to have this opportunity to open ANS 2023 and to convey to you my wishes for the complete success of this conference. I would like to invite you all to contribute to the success of this conference by your participation and discussion, and wish you all inspiring lectures, informative talks and a pleasant stay in Donovaly.

doc. RNDr. Iveta Dirgová Luptáková, PhD.

The Dean of the Faculty of Natural Sciences
University of Ss. Cyril and Methodius in Trnava, Slovak Republic

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Chemistry and Environmental Science

Effect of superabsorbent polymers application on crop growth and uptake of microelements

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Abstract: In recent years, attention has been drawn to the application of superabsorbent polymers (SAPs) as a tool for drought stress mitigation in agriculture. This work investigated the effect of SAPs applied on the seeds of selected plants in the form of thin films (Agro Aquaholder Seed+, PeWaS Ltd.) on crop growth and uptake of microelements. Seeds of barley variety BOJOS, maize var. ALOMBO, rapeseed var. CORZAR, and wheat var. LUANA treated or untreated with SAPs and/or fungicide were planted and grown in two experimental plots located in the Slovak Republic (Borovce) and the Czech Republic (Žabčice) during the years 2021 and 2022. After approx. 6 weeks, plants were harvested, divided into aerial parts and roots, and analysed gravimetrically and by ICP-MS for microelements Co, Cu, or Zn uptake. Both localities of experimental plots were similar in terms of soil chemical parameters, such as TOC, content of K, P, Co, Cu, and Zn (Borovce – 1.89 %, 1.90 %, 0.090 %, 11.5 ppm, 23.8 ppm, and 76.3 ppm; Žabčice – 1.62 %, 2.21 %, 0.105 %, 13.8 ppm, 29.1 ppm, and 96.9 ppm). The years evaluated differed in the level of drought, within the both localities reduced soil moisture or incipient drought in 2021 was described, but in 2022 moderate to severe drought was identified (data from <https://www.intersucho.sk/>). In 2021, a statistically (at $p < 0.05$) significant positive effect of SAPs without or with fungicide application on crop growth was only observed for the Borovce locality and crops of barley and maize. In the following year 2022, when spring was characterised by a severe drought, a statistically positive effect on the crop growth was observed for seeds of maize coating with SAPs at both localities. For all crops evaluated, the uptake of microelements decreased in the order: Zn > Cu > Co. The highest Zn uptake of 71.0 ppm was observed for plants of wheat and decreased in the order: wheat > barley > maize > rapeseed. In the case of Cu and Co, the highest uptake values were 20.4 ppm and 4.09 ppm, respectively, determined at maize. The values of transfer factors (TFs) were in the range of 0.02 – 0.34 for Co, 0.32 – 0.75 for Cu, and 0.43 – 0.90 for Zn. In terms of SAPs application, there were no statistically significant differences in the uptake of microelements and their translocation to aerial parts of plants

Keywords: superabsorbent polymers, soil, drought, crop growth, microelements, uptake

Acknowledgement: This work was supported under the Interreg V-A SK-CZ Programme and project “Využitie superabsorpčných polymérov (SAP) ako inováčného nástroja na zmiernenie dopadov klimatickej zmeny v poľnohospodárstve”, No. 304011Y185, co-financed by the European Regional Development Fund.

Advancing cadmium quantification in cellular compartments: a radioanalytical approach

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Abstract: Distribution and allocation of metals within different cellular compartments significantly impact plant responses to toxic elements like cadmium. While techniques like atomic absorption spectrometry are valuable for subcellular cadmium detection, they require substantial biomaterial quantities, making them less feasible for early developmental stages where sample sizes are limited. In response to this challenge, we have developed a radioanalytical method that allows for precise cadmium quantification in individual cellular compartments using much smaller tissue samples. By focusing on early developmental stage wheat, we analyzed the subcellular accumulation of cadmium using gamma spectrometry. This technique enabled us to study cadmium amounts in tissue samples derived from only 1-3 plants, consisting of tens of milligrams of fresh weight. The approach enabled investigating distribution of cadmium in wheat and revealed a strong correlation between subcellular metal accumulation and specific physiological and biochemical indices. These findings provide valuable insights into the sensitivity and tolerance of wheat to cadmium toxicity. Such knowledge is crucial for developing strategies to mitigate the adverse effects of metal toxicity, particularly in crops intended for organic farming. Ultimately, our approach opens new avenues for investigating metal accumulation dynamics in plants, facilitating the development of resilient and environmentally sustainable agricultural practices.

Keywords: bioaccumulation, cadmium, metal uptake, radioactive tracer, transport

Acknowledgement: The research is supported by the projects APVV-21-0504 and KEGA 022UCM-4/2021.

The impact of poly-3-hydroxybutyrate in soil on its biochemical properties after eight-week pre-incubation and eight weeks of plant growth under different soil-sand ratios

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Abstract: Poly-3-hydroxybutyrate (PHB) is a bacterial biopolymer used for production of biodegradable plastics, environmentally friendly alternative to traditional, long-persisting plastics. This study examined the effects of PHB addition and dilution of soil with sand on soil biological properties those related to soil microbial composition, enzymes and soil respiration. The effects of PHB addition on plant biomass were also compared. The results showed that the PHB addition significantly retarded the plant growth as indicated by reduced dry plant above and below ground biomass (in average by -79% and -91% compared to biomass in unamended soil). However, the addition of PHB to sand:soil mixture in various ratios enhanced the N and K concentrations in plant biomass (in average +55% and +5%) in comparison to the content in sole soil. PHB addition stimulated N and P acquiring enzymes urease and phosphatase (in average by +83% and +69%) compared to unamended soil. Moreover, the soil basal and substrate-induced respirations were higher under PHB addition, however, further varied depending on sand:soil ratio. The results indicated that while soils may be able to break down bioplastics,

Keywords: biodegradable plastics, soil enzymes, soil respiration, plant biomass, plant nutrient content

Properties and benefits of sewage sludge-derived biochars

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Abstract: Pyrolysis represents promising thermochemical method for the processing of complicated waste such as sewage sludge. The thermochemical conversion reduces the total volume of sludge produced by WWTPs. Moreover, pyrolysis transforms sludge into valuable product in compliance with the objectives of the circular economy. However, despite the significant benefits of sludge-based biochar (high content of organic C, Zn, P), its use as a fertilizer has several limitations, mainly due to the relatively high heavy metals content in its structure. In present work we focused on the characterization of industrial sewage sludge-derived pyrogenic materials produced by slow pyrolysis (60 min) at pyrolysis temperatures of 400°C, 550°C, and 700°C. The pH values, ash content, C_{total}, or total Zn concentration in the samples increased with increasing pyrolysis temperature. The concentration of H₂O-extractable Zn in the samples significantly decreased with increasing pyrolysis temperature. The BCR sequential extraction method results demonstrated that with increasing pyrolysis temperature, the bioavailable fractions of Zn (F1, F2) were converted to more stable ones (F3, F4) with low mobility and bioavailability. Based on the results, we can summarize that pyrolysis temperature is considered to be a key factor affecting the overall concentration and chemical speciation of metals in solid pyrolysis products.

Keywords: sewage sludge, pyrolysis, biochar, pyrolysis temperature, heavy metals, Zn

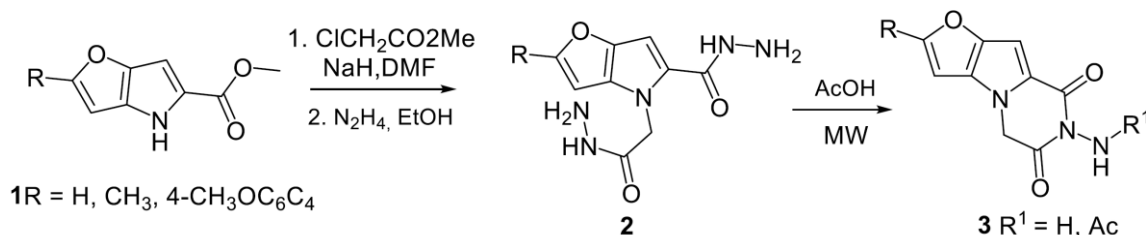
Acknowledgement: This research was funded by the Slovak Research and Development Agency under the contract number SK-AT-20-0004.

Synthesis of tricyclic 5:5:6 heterocycles with three heteroatoms

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Abstract: Furo[2',3':4,5]pyrrolo[1,2-*a*]pyrazines **3** were synthesized from methyl 4*H*-furo[3,2-*b*]pyrrole-5-carboxylates **1** via their alkylation with methyl chloroacetate in DMF/NaH at room temperature overnight, providing methyl 4-(2-methoxy-2-oxoethyl)-4*H*-furo[3,2-*b*]pyrrole-5-carboxylates in 61-67% yields.



Subsequent hydrazinolysis led to the bis-hydrazides **2** in 65-70% yields. Final cyclisation of bis-hydrazides **2** to pyridazine ring can be achieved by heating in acid media. When compounds **2** were irradiated in microwave oven at 180W and 80° C for 35 min, acetamides **3** (R¹ = Ac) were synthesized in 85 - 86% yields. Irradiation of **3** for a shorter period (12 min) at 90 W and 80° C led to the pyrazine **3** (R¹ = H) in 87 % yield.

Synthesized compounds **2** were screened on their antibacterial activity against G- bacterial taxon *Escherichia coli*, CCM 7929 and G+ bacterial taxon *Micrococcus luteus*, CCM 732 compared to the standard 6-aminopenicillanic acid (6-APA).

Keywords: furo[3,2-*b*]pyrrole, alkylation, hydrazine, antibacterial activity

Effect of various organic amendments on soil parameters of Central European Cambisol

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Abstract: Organic amendments (compared to mineral fertilizers) increase soil quality, nutrient content, and biological diversity and abundance in soil, and consequently plant health and crop yield and quality. Amendments derived organic waste materials by pyrolysis (i.e. biochar) or by modification of conventional farmyard manure (via additive to manure fermentation) represent an efficient alternative to traditional livestock waste-derived fertilizers. An effect of three different organic amendments - conventional manure (CM), mineral-based activator-treated manure (MBA-CM), biochar (BA) - and the mineral fertilizer (NPK) on chemical and biological soil parameters of a Cambisol soil was tested in a 3-year small-scale plot field experiment in temperate zone lowland area. All four experimental variants exerted significant differences in pH, dehydrogenase activity (DHA), organic carbon content (Corg), humic/fulvic acid (HA/FA) ratio, and the total, bacterial and fungal phospholipidic fatty acid content. The highest microbial abundance (+114%), Corg (+46%), and HA/FA (+7%) compared to NPK was detected in the soil amended with MBA-CM. Variable beneficial effect (compared to NPK fertilized) of different organic amendments on quality parameters of the most abundant soil type in the Czech Republic was evidenced. Mineral-based activator of biological transformation for improved effect of produced cattle manure on soil quality was valuated.

Keywords: manure, mineral manure activator, biochar, soil microbial biomass, microbial diversity, organic carbon

Accumulation of metals by celery and maize seedlings under hydroponic conditions: the role of transpiration and metal speciation

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Abstract: Metal uptake by crops have been demonstrated to be highly variable and depends on many factors in addition to the metal of interest. The aim of this work was to evaluate the accumulation of Zn, Co, Cd, Cs, or Sr by seedlings of celery (*Apium graveolens* L. var. *rapaceum* Mill.) and maize (*Zea mays* L. convar. *saccharata* Koern.) grown in diluted Hoagland medium (HM) spiked with ⁶⁵ZnCl₂, ⁶⁰CoCl₂, ¹⁰⁹CdCl₂, ¹³⁷CsCl, or ⁸⁵SrCl₂ and the effect of transpiration and metal speciation on these processes. The kinetics of Cs⁺ ions accumulation by maize plants had a linear pattern and correlated with the transpiration rate. The accumulation of Zn²⁺, Co²⁺, Sr²⁺, and Cd²⁺ ions by maize and celery plants did not show a linear course identical to that of transpiration. In addition, during 8 d of cultivation, the volumetric activity of ⁶⁵Zn, ⁶⁰Co and ¹⁰⁹Cd solution uptaken by the plant was higher than the volumetric activity of the HM. This indicates that in addition to the processes of metals uptake by the transpiration stream, the processes of adsorption and selective membrane transport of the abovementioned metals by the root system are also taking place. Root-to-shoot translocation of the studied metals decreased in the order: Cs > Sr > Zn > Cd > Co. Complexing agents, ethylenediaminetetraacetate (EDTA) and nitrilotriacetate (NTA), in the HM reduced Co uptake by the root system of celery. In the presence of an equimolar amount of NTA to CoCl₂ (10 μmol/dm³), a 5-fold lower amount of Co uptaken by the plant in the comparison with celery plants cultivated without the presence of NTA. In the case of Sr and Cd, this effect was not observed. However, a positive effect of EDTA on Cd translocation and NTA on Co translocation was observed. In the presence of an equimolar amount of NTA to CoCl₂ (10 μmol/dm³), Co translocation from celery roots to the aerial parts increased 3-fold compared with the control. Equimolar amounts of EDTA to CdCl₂ (10 μmol/dm³) caused that Cd translocation was increased 1.4-fold compared with the control. The presence of EDTA, NTA, and citrate had no significant effect on Sr translocation from celery and maize roots. Speciation analysis using MINEQL+ software revealed that in the case of Co and Cd, but not for Sr, in the presence of EDTA, NTA, and citrate, the proportion of their bioavailable M²⁺ ionic forms in the HM decreased significantly in favour of [M-NTA]⁻, [M-EDTA]²⁻, or [M-Cit]⁻ complexes.

Keywords: metals, accumulation, celery, maize, transpiration, speciation

Acknowledgement: This work was supported under the Interreg V-A SK-CZ Programme and project “Využitie superabsorpčných polymérov (SAP) ako inováčného nástroja na zmiernenie dopadov klimatickej zmeny v poľnohospodárstve”, No. 304011Y185, co-financed by the European Regional Development Fund.

Vortex-assisted liquid-liquid microextraction based on new fluorophore for the determination of anionic surfactants in water samples

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Abstract: A new green, ultrasensitive and selective method based on vortex-assisted liquid-liquid microextraction (VALLME) was developed for the spectrofluorimetric determination of sodium dodecyl sulphate (SDS) using the new fluorophore 3,3'-diethyloxadicyanine iodide (DODCI). The principle of the method developed by us consists in the reaction of SDS with DODCI at pH 3, followed by VALLME of the formed ionic associate (IA) into the organic phase containing n-amyl acetate. Fluorescence intensity was measured in the wavelength range 600-800 nm at an excitation wavelength of 640 nm with a peak around 668 nm. The linearity of the calibration dependence was observed in the concentration range of SDS from 0 to 2.6 ng mL⁻¹ ($R^2 = 0.9980$). The limit of detection (LOD) were 0.10 ng mL⁻¹. The accuracy and correctness of the proposed method was verified during two consecutive days with RSD values of 2.6-3.7% and recovery of 93.5-107.9%. To demonstrate the practicality of the proposed procedure, a method was developed and applied to the determination of SDS in real water samples and pharmaceutical tablets. Satisfactory recovery data were obtained, ranging from 93.1 to 109.0%, with a relative standard deviation of 2.2 to 4.9%.

Keywords: anionic surfactants, microextraction, spectrofluorimetry, green chemistry

Acknowledgement: Yaroslav Bazel' and Sofia Kakalejčíková thanks the Scientific Grant Agency VEGA of the Ministry of Education of the Slovak Republic and the Slovak Academy of Sciences for their support (Grant no. 1/0177/23).

Determination of para-anisidine by HPLC method using azo coupling reaction

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Abstract: Para-anisidine (PA) or 4-methoxyaniline is used as an insect repellent and ovicide. Its derivatives are also widely used in chemical reactions as intermediates for the production of target materials, such as pharmaceuticals, dyes, perfumes, photoinitiators, etc. PA is colorless crystals that easily oxidize and darken in air, have no smell.

To determine residual amounts of PA, derivatization was performed to form an azo compound. To study this effect, the derivatization reaction was performed in a broad range of hydrogen ion concentration between pH 3.4 to 13.5. Another important factor for the formation of the azo compound is the concentration of reagents. In our experiments the concentration of diazonium cation varied from 1 to 30 fold higher amounts relative to the PA amount.

The structure of the synthesized triazene was also confirmed by IR-spectroscopy due to stretching vibrations of hydrogen atom bonded to a nitrogen atom in the triazene >N-H group. The linear dependence of the chromatographic peak area on PA concentration was observed. Based on the obtained data, the method was optimized to determine PA in soils and wastewater using high performance liquid chromatography, and tested on model samples and real objects.

Keywords: para-anisidine, azo coupling reaction, HPLC determination

Avenanthramides as potential pharmaceuticals and their occurrence in different genotypes of *Avena* spp.

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Abstract: Avenanthramides (AVNs) are promising secondary metabolites specific to *Avena* spp. (oat) - amides of anthranilic acid linked to various polyphenolic acids. These natural compounds have been reported to exert numerous biological effects. POM analysis and similar approaches are significant tools based on calculating various physicochemical properties predicting biological activity, ADME parameters, and toxicity. These methods are used to evaluate a molecule's potential to become a drug candidate. The evaluation of primary in silico parameters revealed significant differences among individual AVNs, highlighting the most promising candidates, f.e. AVN C (2c). These preliminary results may help coordinate and initiate other research projects focused on particular AVNs, especially those with predicted good bioactivity, low toxicity, optimal ADME parameters, and perspectives. Another goal was to find a suitable biological source of these substances. We investigated the content of avenanthramides in the grain of different oat genotypes, grown and harvested in Slovakia in the Vígľaš-Pstruša location on isolated fields. A separation method - high-performance liquid chromatography with DAD detection on a column with a reverse arrangement of phases of the C18 type (RP-HPLC-DAD) turned out to be a suitable analytical method for the determination of AVNs. High resolution mass spectrometry (HRMS) confirmed the presence of avenanthramides AVN A (2p), AVN B (2f) and AVN C (2c), three major avenanthramides in selected oat genotypes. Selected varieties with a high content of AVNs may be suitable for further research, including methods to effectively increase their amount such as germination and different elicitation techniques. Such genotypes may also be suitable for the production of functional foods and for the pharmaceutical industry.

Keywords: food, oat, avenanthramides

Acknowledgement: This work was supported by grants No. SRDA-17-0113, SRDA-20-0413 and KEGA 025UCM-4/2021.

Influence of surfactants on arsenic bioleaching from mining wastes

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Abstract: Heavy metal contamination of the environment is particularly problematic in former mining areas. In Poland, one of the old arsenic-gold mining and processing centres is Złoty Stok in the southwest of the country. Ore mining and processing, which took place in the area of Złoty Stok, generated large amounts of waste materials rich in As, such as mine waste rock, slag, and tailings. Most of the mine spoils are hardly distinguishable from the natural forms of the slopes. It is assumed that about 2% of the total content of arsenic could be leached from carbonates and amorphous Fe oxides under favourable conditions. Therefore, the main objective of the study was to perform fundamental research on mineral-bacteria-surfactant interactions in the context of their role in arsenic release that occurs in the post-mining heaps. Bioleaching of arsenic waste using acidophilic bacteria was carried out in columns to reflect the natural conditions of the heap. Surfactants, including cetyltrimethylammonium bromide and sodium dodecyl sulfate, were adsorbed on mineral waste to change surface properties and define the conditions under which arsenic release is inhibited.

Keywords: arsenic, bio-extraction, cetyltrimethylammonium bromide, sodium dodecyl sulfate, surface modification

Phytomanagement of petroleum-polluted soils with industrial crop *Miscanthus x giganteus*

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Abstract: Petroleum hydrocarbons are one of the most abundant sources of environmental pollution. A series of experiments, both pot and field, were carried out to assess the potential of industrial crop *Miscanthus x giganteus* to grow on petroleum contaminated soils and contribute to their remediation and quality of biomass in terms of its potential valorization.

As expected, higher hydrocarbons concentrations exhibited toxic effects on the plant biomass and physiological parameters, however the toxicity was higher in soils from real older polluted sites compared to diesel-spiked soils indicating significant toxicity synergy of other pollutants, salinity or soil parameters. Different plant parameters (biomass, height, physiological indices and others) responded to hydrocarbon toxicity with different sensitivity. At lower diesel concentrations significant hormesis (temporal increase) was found for some photosynthetic indicators.

Degradation of hydrocarbons followed dominantly the first-order kinetics suggesting ongoing biodegradation. In planted soils degradation was enhanced, however the enhancement was proportional to plant development. So, it was negligible at higher concentrations with the highest toxicity. Since no uptake of petroleum hydrocarbons to above-ground plant parts was detected, this indicates that the most likely mechanisms is the support of biodegrading soil microorganisms by plants, i.e. rhizodegradation. This conclusion is also supported by increased abundance of some petroleum degrading bacteria genera in miscanthus rhizosphere in soil from real contaminated site. On the other hand, no increase in abundance of genes for several enzymes involved in the biodegradation of petroleum was detected in diesel contaminated soil, so the phytoremediation mechanism is still unclear.

Some practical biomass parameters (such heating value or composition of pyrolytic products) were slightly affected in petroleum-contaminated soil, nevertheless the applicability of biomass for energetic purposes was preserved.

Overall, these results indicate feasibility of *M. x giganteus* for phytomanagement of petroleum contaminated sites, however the task is not simple, but it is very site-specific.

Keywords: phytomanagement, *Miscanthus x giganteus*, petroleum contamination, biomass, phytoremediation

Sensing performance of a D-shaped optical fiber with perspective of water contamination testing

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Abstract: A novel D-shaped optical fiber is used in this work as chemical sensor expressing sensitivity on water contamination. Thanks to the special fabrication process, the fiber holds the D-shaped cross section along its whole length. The evanescent wave interaction of the transmitted laser radiation with liquid analyte in the near infrared region resulted any transmission changes in the case of water. On the other hand, applying isopropanol in the sensing region of the fiber resulted in significant increase of the transmitted intensity and change of the output beam shape from elliptical to more circular one. Analysing the physical mechanism of the evanescent wave interaction at the flat fiber surface, both enhancement and reduction of the individual guided mode transmission was identified with increasing refraction index of the analyte depending on the character of the mode. Measurement of isopropanol concentration in water solvent is demonstrated using the introduced fiber with perspective of further increase of the concentration sensitivity.

Keywords: fiber optics sensor, D-shaped fiber, evanescent wave interaction, contaminant concentration measurement

Acknowledgement: This work was supported by Slovak Scientific Grant Agency through grant No. VEGA2/0070/21 and VEGA1/0195/23.

Utilisation of microextraction technique for preconcentration and determination selected xenobiotics in fruit using GC-MS

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Abstract: The analysis of foods and related products can be regarded as an important topic in the analytical chemistry. Chromatographic methods play an important role in the analysis of complex mixtures such in food analysis. Food ingredients have to be determined for the reason of quality assurance, or contaminants of foods as well as food adulteration must be controlled. Most food samples have to be understood as complex mixtures of a variety of different components.

The analytes of the interest have to be separated from interfering matrix components before determination. From xenobiotics occurred in fruits pesticides were chosen for this study. In the analysis of pesticide residues in fruit various substances have been determined at very low concentration.

The main objective of this paper is validation of the method for the determination of pesticides in non-fatty food using the environmentally friendly extraction technique known as stir bar sorptive extraction (SBSE), followed by liquid desorption in a solvent and fast capillary gas chromatography–mass spectrometry with quadrupole detector. Optimization of the method was obtained. The optimized method for non-fatty food sample preparation was validated and applied to analyses to real samples. Limits of quantification were established deeply under the concentration level 5 µg/kg. (Maximal residual limit specified by EU Commission is 10 µg/kg.)

Keywords: GC-MS; xenobiotics; microextraction techniques

Acknowledgement: This study was realized with support of project KEGA 022UCM-4/2023.

Determination of biogenic amines in food by HPLC

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Abstract: Biogenic amines (BAs) are low-molecular-weight nitrogen compounds of various structures containing characteristic amino-group. They are formed primarily by the decarboxylation of amino acids by microbial enzymes. Most of them have strong physiological effect and play an important biological role as sources of nitrogen and precursors for synthesis of hormones, alkaloids, nucleic acids and proteins. Small amounts of BAs are generally bio-synthesized in plant and animal cells and large quantities are found as a consequence of microbial metabolism in fermented foods such as sausages, fish products, cheese, fermented vegetables, and beverages (beer, ciders and wine). However, they are toxic if consumed in large quantities. Therefore, the development of methods sensitive to determine these substances are very much needed. The biogenic amines often analyzed in food, are histamine, tyramine, putrescine, cadaverine, spermine, spermidine, tryptamine and phenylethylamine. Chromatographic methods are often used for determination of BAs. High performance liquid chromatography (HPLC) for the simultaneous determination of eight BAs with derivatization step and UV detection is presented here. Samples of food, as vegetables, meat, meat products, and fish were extracted with 10% TCA, and then filtered through a membrane filter. As a derivatizing reagent was used dansyl chloride. Then the samples were evaporated and dissolved in acetonitrile again. HPLC analysis was performed on a reversed phase column Hypersil BDS C18 with the mobile phase of 0.02 M acetic acid, and acetonitrile. Samples were detected at 254 nm. Their amount increases in direct proportion with microbial fermentation. Interests are mainly in terms of medicine, but mainly food. Since biogenic amines are biologically active substances with significant effect on human health, it is necessary to control the concentrations of these substances in foods.

Keywords: biogenic amines, liquid chromatography, determination, food

Acknowledgement: Supported by Kega 025UCM-4/2021.

Benthic diatoms as bioindicators in constructed wetland

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Abstract: The diversity of diatom communities was used to assess water quality after implementing the Wetland+® technology for treating water contaminated with toxic hexachlorocyclohexane (HCH) (Hájek, Czech Republic). Wetland+® system consists of an aeration and sedimentation module, a permeable reactive barrier, a biosorption module, and an aerobic wetland system. Benthic diatoms are microscopic algae (*Bacillariophyceae*) that are common in almost all types of water. As diatoms are sensitive to many different environmental factors, they are very good bioindicators of changes in the water environment. In this study, the Specific Pollution Sensitivity Index (IPS) and the Shannon Diversity Index (SDI) were used to define the water quality based on the diatom species counted using the OMNIDIA software (France). Diatoms were analyzed in Wetland+® biosorption and aerobic wetland modules and in profiles of the Ostrovský Creek, the recipient of the Wetland+® outflow. More diatom species were observed in sites further from the source of HCH pollution than in sites closer to the beginning of Wetland+® as well as in the Ostrovský Creek. To conclude, diatom diversity was in line with water quality based on chemical parameters. The advantage of using a diatom community is in assessing the water quality within the longer term, compared to assessment based on physicochemical parameters that change more quickly.

Keywords: diatoms, biomonitoring, constructed wetlands, hexachlorocyclohexane

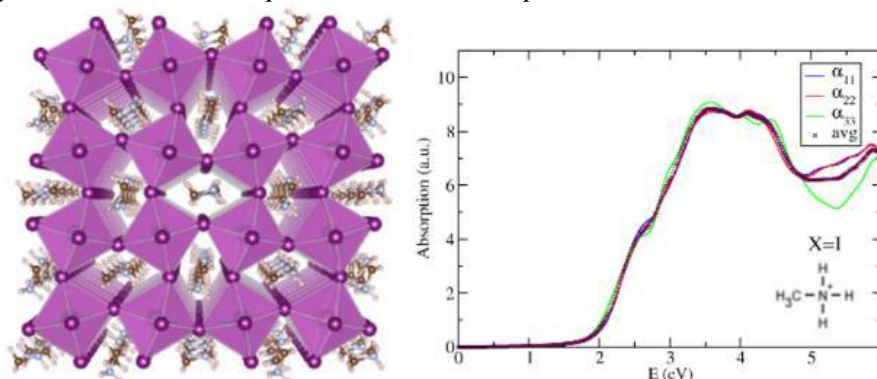
First-principles modelling of organic-inorganic perovskites for photovoltaic applications

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Abstract: Hybrid organic-metal halide perovskites (PV) attracted much attention as promising and technologically cheap materials in field of light harvesting applications due to their quality optoelectronic properties and the apparent ease of implementation as absorbers in highly efficient photovoltaic devices. The PVs typically have crystal structure composed of three primary ions with a stoichiometry of ABX₃, where A-cation can be methylammonium (MA) or formamidinium (FA), and either lead or tin are the B cation, with halides: chlorine, bromine or iodine as the X anion. The optical transitions in PV's active layers crucially determine their optical absorption properties to a large extent. Sub-bandgap absorption of incident photons in the PV can result either from thermal disorder or from structural imperfections. The charge recombination processes play a significant role in restricting the performance of perovskite-based applications and can be influenced also by the presence of defect states. We will briefly demonstrate methodology based on quantum chemistry and the Density Functional Theory (DFT) approaches to investigate the key chemico-physical features of PVs, underlying physics of defects, charge distribution, electronic band structure and lattice dynamics. Such computational frameworks represent a viable support not only to measurement techniques but to effective PV photovoltaic devices fabrication.



Keywords: hybrid metal halides, perovskite structures, photovoltaic, electronic bands, DFT

Acknowledgement: This research was partially supported by the Slovak Research and Development Agency No. APVV SK-CZ-RD-21-0043 and Slovak Scientific Grant Agency VEGA No. 2/0055/21. We acknowledge PRACE for awarding access to the Fenix Infrastructure resources at [TGCC Irene], which are partially funded from the European Union's Horizon 2020 research and innovation programme through the ICEI project under the grant agreement No. 800858.

DITHIOXAMIDE – an UNEXPECTED “CHAMELEON” in the FIELDS of CHEMISTRY

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Abstract: Research is forced by an urgency to answer a question, that have been asked not long time ago. While focusing on a crucial role of the dithioamide (DTO) in (cyclo)condensation step of the Ketcham reaction (Figure) [1,2], the remark from the audience, if I am sure that DTO with properties of amides can do that, came out. Since it is obvious that for the amides as being the functional derivatives of carboxylic acids with -HN(C=O)- linkage, the condensations (A_d - E) are not possible contrary to the simple amines (1° - NH_2 or 2° - NH-), DTO with a $\text{H}_2\text{N(C=S)}$ structural fragment should stay untouched as well. Unless... Due to the electron-donating character of both functional groups – either the nitrogen atom from the terminal NH_2 or sulphur atoms in the vicinal C=S in =C-SH array, the bipolar character in the structure of DTO is maintained in its tautomeric form. Such structural arrangement is responsible for the reactivity of DTO according to the A_d - E manner. Phenomenon is supported by the structure of known coordination compounds with DTO acting as the ligand possessing combined $\text{S=C-NH}_2 \leftrightarrow \text{HS-C=NH}$ mode (Figure) [3].

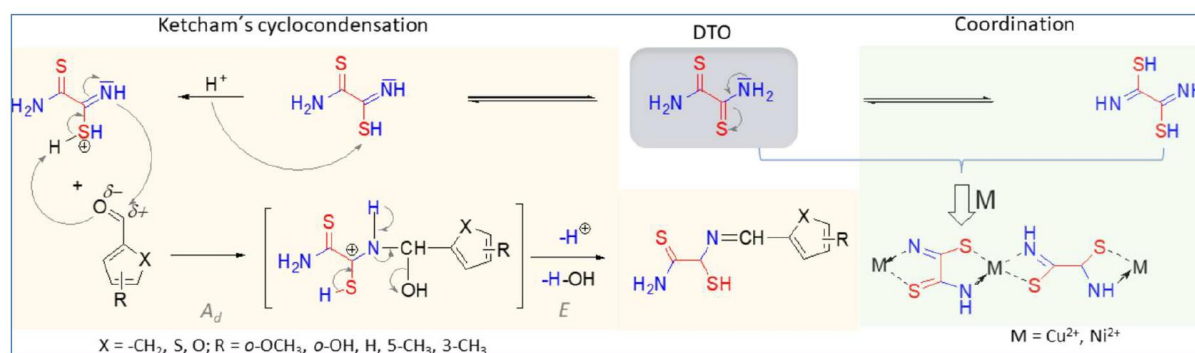


Figure. Role of dithioamide (DTO) in organic synthesis (Ketcham's reaction) and in inorganic and analytical chemistry (coordination and detection of copper and other metal ions).

Keywords: dithioamide (DTO), condensation, (tio)oxo-(tio)enol tautomerism, Ketcham reaction, coordination

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Acknowledgement: Supported by SK Ministry of education VEGA 1/0086/21 and SK Research agency APVV-19-0087.

Effect of soil nutrients on the stability of superabsorbent polymers: hydrogel swelling and potassium release

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Abstract: Superabsorbent polymers (SAPs) represent a potential tool to mitigate drought stress in agriculture due to their excellent water absorption and water retention properties. The aim of this work was to evaluate the effect of soil nutrients, especially alkali metals and microelements, on hydrogel swelling and potassium release as an important macroelement in plant nutrition. For these purposes, a commercially available superabsorbent polymer Aquaholder® Seed (PeWaS Ltd., Slovak Republic) designed for agricultural applications was used. All experiments were carried out under laboratory conditions and using flame photometry. The studied polymer contained K in mass fraction of 12.0 %, as determined by flame photometry and also confirmed by measurement of ⁴⁰K isotope using scintillation gamma-spectrometry. Application of deionized water and solutions with equimolar amounts of Na, Cs, Zn, Cu, Co, and Cd to the K present in the polymer resulted in the release of K from the polymer in the amounts of 14.2 %, 34.2 %, 31.4 %, 48.0 %, 67.0 %, 43.7 %, and 76.2 %, respectively. Hoagland's medium (HM) solutions of 100 % or 10 % strength mimicking the soil solutions were also used in this series of experiments. When 100 % HM was applied, K release was 47.4 % and when the SAP-SEED polymer was treated with 10 % HM solution, 17.4 % of K was released from the polymer. In the case of application of solutions containing Na, sodium binding was evaluated in addition to K release. It was found that when equimolar amounts of Na and solutions of 100 % HM and 10 % HM were used, Na binding by the polymer was 30.8 %, 22.8 %, and 59.0 %, respectively. In these cases, the molar ratios between the amount of K released and the amount of Na bound were 0.63, 1.44, and 0.62, respectively. Hydrogel formation or swelling in the presence of equimolar amounts of Na, K, Cs, Zn, Cu, Co, and Cd to the K present in the polymer or in the presence of 100 % HM and 10 % HM solutions in the comparison with the control (hydrogel prepared in deionized water) decreased in the following order: deionized water (100 %) > 10 % HM (69.3 %) > K (60.1 %) > Cs (60.0 %) > Na (57.3 %) > 100 % HM (18.8 %) > Co (16.2 %) > Cd (12.8 %) > Zn (12.4 %) > Cu (6.5 %).

Keywords: superabsorbent polymers, agriculture, alkali metals, microelements, potassium release, hydrogel swelling

Acknowledgement: This work was supported under the Interreg V-A SK-CZ Programme and project “Využitie superabsorbčných polymérov (SAP) ako inováčného nástroja na zmiernenie dopadov klimatickej zmeny v poľnohospodárstve”, No. 304011Y185, co-financed by the European Regional Development Fund.

Iron complexes with different amino acids

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Abstract: Iron is an important element involved in many biochemical reactions in the human body, including oxygen transport, energy production and many other important processes [1]. From bioinorganic aspects iron reaction with amino acids are essential, because they help us to clarify the existence of some serious diseases. The aim of this work was to study the reaction of iron compounds and with selected amino acids and the study of the influence of experimental conditions on the composition of the product. The study of iron complexes formation with different amino acids has shown, that the composition of the final products are rather complicated due to redox reactions that in oxygen presence finally led to iron oxides formation [2].

Keywords: iron, amino acid, synthesis of iron-aminoacid complexes

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Acknowledgement: Slovak grant agencies (VEGA 1/0086/21) are acknowledged for the financial support.

Diversity of wheat in accumulating essential metal ions for organic farming: a comprehensive study of micronutrient enrichment

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Abstract: The global population faces a significant challenge due to widespread micronutrient deficiencies, negatively impacting millions' health and well-being. The nutritional quality of modern wheat varieties has declined compared to traditional landraces, exacerbated by increasing grain production. Enriching cereal grains, especially wheat, with essential micronutrients like zinc is a primary focus of current research. This study analyzes over 70 wheat cultivars to address micronutrient deficiencies. Evaluating phenotypic, metabolic, and genetic diversity, we assess their ability to accumulate specific micronutrients in tissues and grains, with a particular focus on zinc—a vital micronutrient for human health. The investigation delves into the mechanisms influencing zinc content variability in wheat tissues. By identifying key parameters, we aim to elucidate zinc uptake and transport processes within plants, facilitating the selection of wheat varieties with higher zinc content for future breeding efforts in organic cultivation. Moreover, this comprehensive study sheds light on the interplay between genetic diversity and micronutrient accumulation in wheat, laying the groundwork for improving grain nutritional quality in organic cultivation systems. Ultimately, this research's outcomes will contribute to addressing global malnutrition and metal toxicity issues, profoundly impacting the well-being of the world's population.

Keywords: bioaccumulation, biofortification, durum wheat, metal toxicity

Acknowledgement: The research is supported by the projects APVV-21-0504 and KEGA 022UCM-4/2021.



Biology and Biotechnology

Phytoremediation potentials of quinoa (*Chenopodium quinoa* Willd) and impacts on human health once cultivated in potential toxic elements contaminated soils

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Abstract: Phytoremediation of potential toxic elements contaminated soils has proved high success and efficiency worldwide. On the other hand, Quinoa (*Chenopodium quinoa* Willd) is recognized as a crop of great value in terms of nutrition and tolerance to cold, drought and saline stress. Recently, it demonstrated high potentials to be used for energy production (energy value 18.27 MJ.kg⁻¹). Nevertheless, information about the phytoremediation potentials of this crop is still scarce and requires further investigations. An *ex situ* pot experiment was established by cultivating quinoa crops in soils contaminated with an increasing gradient of potential toxic elements (As, Cd, Pb and Zn). The work aimed at studying the capacity of the crop to grow well and produce biomass that could be valorized commercially in contaminated soils, as well as its potential impacts on human health. It also aimed at studying the impacts of quinoa cultivation on the soils' physicochemical and microbiological parameters. The results showed that the quinoa plants possessed good potentials to grow well and produce biomass in mild toxic elements concentrations and enhance the quality of the degraded soils. Finally, the quinoa showed good phytoremediation potentials, however the risk of the elements' toxicity is challenging for human health.

Keywords: Quinoa, soil contamination, BCF, TF, phytoremediation

Differences in stability and dynamic motion of the N-terminal domain of the human ryanodine receptor 2 induced by central helix mutations

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Abstract: Regular muscle contraction is one of the key processes occurring in all Animalia. Ryanodine receptors (RyRs), the largest ion channels known to date, play a key role in this process. Their main physiological role is to transfer calcium cations into the cytoplasm, thereby triggering a cascade of reactions resulting in muscle contraction [1]. In mammals, three isoforms of this channel have been identified. They are predominantly expressed in skeletal muscle (RyR1), myocardium (RyR2) and different tissues (RyR3). Dysfunction of the RyR2 channel causes serious tachycardias and arrhythmias.

In our laboratory we predominantly carry out structural studies of the human RyR2 isoform (hRyR2) using a combination of “in silico” and “in vitro” approaches. We have determined the crystal structure of the N-terminal domain of hRyR2. To better understand the role of several residues known to be associated with arrhythmias, we purified and biophysically characterized the I419F, R420W and L433P mutants, which occur in the central α -helix, and S616L, which is part of the suspected dantrolene binding site. Extensive molecular dynamics studies showed that the I419F, R420W and L433P mutations influence the dynamics of the RyR2 channel opening and closing and therefore, at least in part, may disrupt the regular release of Ca^{2+} from the sarcoplasmic reticulum.

Keywords: human ryanodine receptor 2, N-terminal domain, thermal stability, molecular dynamics

Acknowledgement: This work was financially supported by Slovak Grant Agency VEGA, grant no. 2/0131/20.

Genetic diversity of the *Ganoderma* species in Central Europe

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Abstract: *Ganoderma* (Basidiomycota) is a cosmopolitan wood-decay polypore causing white rot of a wide range of woody plants. It plays an important role in the process of wood decomposition in forest ecosystems, but it also known as a dangerous phytopathogen. Although the genus has been sampled for molecular phylogenetic studies worldwide, available data from Central Europe are limited. The field research was carried out during the years 2015-2018 in Slovakia and Czech Republic (Moravia). *Ganoderma* species were identified by sequence analysis of selected DNA markers (ITS, 25S LSU, *tef-1α*). According to phylogenetic analysis of ITS sequences 75 basidocarps were divided into 6 clades: *Ganoderma applanatum*, *G. adspersum*, *G. pfeifferi*, *G. resinaceum*, *G. carnosum*, *G. lucidum*. Very low genetic diversity between *G. lucidum* and *G. carnosum* clades and the existence of 2 previously unrecognized genotypes in *G. resinaceum* clade was observed. The genetic non-homogeneity of *G. resinaceum* was confirmed by *tef-1α* gene sequence analysis. The observed diversity between 2 genotypes of *G. resinaceum* was 0.0304 base substitutions per site, two times higher than diversity between *G. lucidum* and *G. carnosum* clades (0.016). The rare species *G. valesiacum* was not recorded by field research during our study.

Keywords: molecular diversity, intraspecific variability, interspecific variability, ITS, *tef-1α*, wood-decay fungi

Acknowledgement: This work was funded by KEGA Grant No. 014UMB-4/2023 and VEGA Grant No. 1/0564/21 and by the ITMS Research & Development Operational Programme; ERDF, Grant/Award No. 26210120024.

Residues of pharmaceuticals and industrial substances in substrates based on treated sewage sludge and the substrates use in forestry and arboriculture

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Abstract: Sludge produced in sewage treatment plants constitutes an abundant source of waste material. Properly treated, it can be reapplied especially as part of growth substrates. In the Czech Republic, it is forbidden to process sewage sludge for food production, due to the content of substances dangerous to human health. Despite being rich in plant-usable soil nutrients such as carbon, nitrogen, potassium, phosphorus, calcium and magnesium, it may contain many potentially dangerous substances, e.g. heavy metals, bacteria, viruses, antibiotics, synthetic hormones and other drugs, polychlorinated biphenyls, polycyclic aromatic hydrocarbons, etc.

The content of potentially harmful substances can be significantly reduced by controlled composting based on governmentally approved methodology complying with the legislative limits of sludge use as the basis of growth substrates for other purposes excluding foodstuff. The study compared the contents of pharmaceutical and industrial residues, specifically 51 substances, divided into 7 groups: 6 pharmaceutical groups with a pronounced effect on human health and 1 collective group of industrial substances. The contents were compared among three different substrate mixture variants (var 1–5) before composting and after the first and the second composting. Biomass of lettuce *Lactuca sativa* L., grown on respective substrates was also analysed for the total contents of dangerous substances. Before composting, the highest contents were found in the cases of C-pharmaceuticals affecting the cardiovascular system, M-pharmaceuticals affecting the musculoskeletal system and R-pharmaceuticals affecting the respiratory system. After the first composting, a significant reduction in the contents of most of the analysed pharmaceuticals and industrial substances was observed (by up to 50% on average), whereas in most cases the content further decreased with the second composting.

However, after the second composting, the reduction in content was no longer so significant, as some groups of pharmaceuticals in several substrate variants slightly increased backwards. Tests in the lettuce biomass detected significant amount of N-pharmaceuticals (affecting the nervous system), M-pharmaceuticals and industrial substances that the plant absorbed from the substrate var 1 after both first and second composting, and N-pharmaceuticals and J-pharmaceuticals (antibiotics) in the substrate var 2 after the first composting.

Substrate production technology was proposed as part of the project implementation. In addition to peat, bark and wood substrates, the production process involved stabilized and composted sludge, granulated glauconite and biochar. Modified glauconite was added as a significant natural potassium source, biochar as dangerous substances sorbent and a large pool of sequestered atmospheric carbon and additional nutrients. Two substrate prototypes were produced according to the approved technology: organo-mineral designed for planting forest trees seedlings and structural for adjusting the rooting area and outplanting trees in urban areas. Substrate trials are currently ongoing on several experimental sites. The organo-mineral substrate was used during forest recultivation at the Hrbov-Lhenice mining site, where it was locally added to individual seedling planting spots. Further experiments were established in forest nurseries, e.g. at the Training Enterprise Masarykův les Křtiny or in Planá nad Lužnicí, where the substrate was applied directly to seedling beds. The second substrate devised for arboricultural practice was applied in the Tisimice orchard, the only research plot of its kind in the Czech Republic, to fill outplanting pits of small-leaved linden (*Tilia cordata* L.).

Keywords: extremophiles, NaCl, halophile, hypersaline environments

Life on the edge: salt tolerant cyanobacteria

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Abstract: Naturally occurring mineral sodium chloride (NaCl) is essential for life. Concentrations of NaCl in the environment can vary significantly depending on the studied location. Both aquatic and terrestrial biotopes represent hypersaline environments. These worldwide biotopes host halotolerant and halophilic organisms primarily adapted to live in the environment with high salinity. Many microorganisms adapted to environments with high salinity are phototrophs, especially cyanobacteria. They adapted using a "salt-out" adaptation strategy, accumulating osmolytes in the cytoplasm and removing salt cations from the cells. This maintains the osmotic balance in the cells. The most common halotolerant cyanobacteria are *Cyanothece halobia*, *Aphanothece halophytica*, *Halospirulina tapeticola*, *Dactylococcopsis salina* and *Halomicronema excentricum*. Their ability to synthesise a wide range of potentially valuable substances predisposes them to relatively widespread use in biotechnology. The study overviews the world's saline habitats and microbial communities. It presents the species of cyanobacteria that colonise them. Our project also analyses and summarises most common life strategies cyanobacteria use to adapt to life in salty habitats.

Keywords: extremophiles, NaCl, halophile, hypersaline environments

Overexpression of oak dehydrin gene in tobacco enhances tolerance to copper stress

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Abstract: The dehydrin gene *QDhn3* from *Quercus robur L.* driven by the constitutive double *dCaMV 35* promoter was introduced into tobacco via *Agrobacterium*-mediated transformation. Transgenic and non-transgenic (control) seeds were germinated in the presence/absence of 50 mM CuCl₂ for 21 days. Transgenic seedlings showed significantly higher contents of photosynthetic pigments and osmoprotectant proline compared to non-transgenic seedlings, when exposed to Cu. Real time PCR analyses revealed that an overexpression of the *Dhn3* gene altered the expression of antioxidant enzymes, PR proteins and some metal transporters responsible for heavy metal detoxification and sequestration, in non-stressed as well as in Cu-stressed seedlings. These results indicate that the dehydrin *Dhn3* might be involved in plant response to heavy metals.

Keywords: copper stress, woody dehydrins, *Quercus robur*, transgenic tobacco plants

Acknowledgement: This work was supported by the projects VEGA 2/05258/20, KEGA 001UCM-4/2022 and APVV 20-0413.

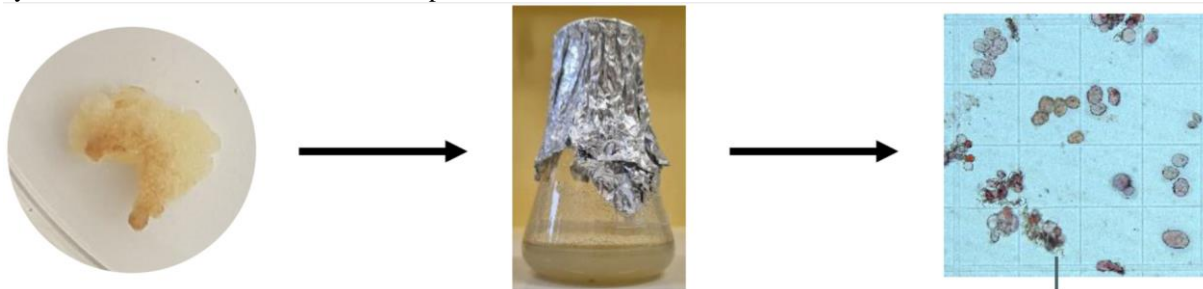
Establishment of callus cell-derived plant stem cells in *Calendula officinalis* L.

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Abstract: Technologies of plant cell cultures in vitro are experiencing a rising interest in chemical compounds produced by plant stem cells and stem cell-like cells, which can be established from tissues containing meristematic cells. This study investigated the establishment of these cells in *Calendula officinalis* L. through induction and growth of callus cell biomass. Different types of explants (leaves and roots) with various combinations of auxins and cytokinins were tested for initiation of callus, growth of sub-cultivated callus biomass, and establishment of stem cells or stem cell-like cells. Our results indicate that the type of explant and the combination of plant growth regulators significantly influence callus induction and growth parameters. However, the most important finding of this study was the confirmation of the presence of stem cells or stem-like cells in the sub-cultured biomass of callus cells by specific vacuole characterisation. In the case of *C. officinalis* L., this study represents the first successful induction and cultivation of stem cells in cell suspension culture. The establishment of in vitro stem cells or stem cell-like cell cultures in *C. officinalis* L. presents opportunities for potential applications in in vitro cultivation systems and alternative uses for this crop.



Keywords: plant stem cells, dedifferentiated cells, callus culture, suspension culture

Preparation of the plant extracts with significant enhanced bio-activity, by application of innovative engine, worked on simultaneous application of several physical factors for new food supplements generation

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Abstract: It has been developed original engine for frugal extraction of plant extractive compounds with accelerating effect, worked upon the principle of the simultaneous combination of several physical factors (sonication, temperature, by electrical field promoting extraction device). By application of this engine, it was obtained plant extract samples with several times enhanced dry matter content as well as bio-activity, particularly antioxidant activity, antibacterial activity, inhibition activity on pathophysiological important enzymes, anti-inflammatory activity etc. This device was utilize in the process of the extract samples preparation. Several prepared samples expressed significant simultaneous antibacterial effect, inhibition activity on Main protease of SARS-CoV-2, antioxidant activity as well as anti-inflammatory activity. Especially these activities expressed following extract samples: from bark of oak (*Quercus robur*, L.), flower of Oregano, *Origanum vulgare*, grains of rapeseed, *Brassica napus*, grains of oat, *Avena sativa*, and others. The enhancement factor (coefficient) warried in interval (2,8 - 6,2). The extraction products were prepared for development of new food supplements for pandemic situation, aimed to enhance defensiveness of human body.

Keywords: physical promotion of extraction process, enhanced bio-activity, food supplements

Acknowledgement: This paper was supported by grant No. SRDA-20-0413.

Two novel closely related subfamilies of the α -amylase family GH13

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Abstract: Within the CAZy database, the main α -amylase family GH13 classifies also characterized amylolytic enzymes that still have not been assigned to any of the established GH13 subfamilies. This is also the case of the α -amylase from *Haloarcula japonica* and the maltogenic amylase from *Thermotoga neapolitana*. The present study delivers a detailed in silico analysis of two mutually related groups of GH13 members represented just by the two above-mentioned enzymes. Interestingly, although both groups share some sequence attributes within the seven conserved sequence regions (CSRs), there are also other features in CSRs that clearly distinguish the two groups from each other. The well-conserved cysteine in the CSR-II positioned just before the catalytic nucleophile is an exclusively shared residue that simultaneously discriminates the novel groups from all 46 GH13 subfamilies established so far. In addition, and among other features, while the hypothetical proteins represented by *H. japonica* α -amylase can be recognized by a well-conserved glutamic acid directly preceding the general acid/base, the members of *T. neapolitana* maltogenic amylase group possess a well-conserved tryptophan at the beginning of the CSR-III. The two groups described here may thus define two novel and closely related, but still independent GH13 subfamilies.

Keywords: α -amylase; maltogenic amylase; GH13 subfamily; sequence-structural features; phylogenetic analysis

Molecular - biological identification and characterization of a new isolate of bean common mosaic virus originated from Slovakia

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Abstract: Bean common mosaic virus from the genus *Potyvirus* has a wide range of hosts and a very negative impact on cultivated crops from the genus *Phaseolus*. The risk of viral infection of economically important crops increases even if the carriers of the virus are related plant species growing on agroecological interfaces. Such plant species have emerged as new hosts for BCMV, usually harboring novel genetic variants of the virus. A novel genetic variant of BCMV was isolated from a symptomatic crownvetch plant (*Securigera varia* L. Lassen), where the presence of this virus was confirmed via Western blot analysis and by amino acid identities in peptide fragments of CI, HC-pro, and CP proteins using the nanoLC-ESI-Q-TOF. The novel BCMV SVK isolate differed from the most genetically similar one in 0.91% of nucleotides and 1.55% of amino acids. The highest number of amino acid substitutions (8.8% of amino acids) was in the P1 protein, followed by CP (2.44% of amino acids). Minor substitutions were in Hc-pro, CI, and Nib proteins. The symptomatic crownvetch plant was confirmed as a new host and carrier of the novel BCMV isolate.

Keywords: BCMV, genome, new isolate, amino acid substitution

Acknowledgement: This research was supported by the Slovak Research and Development Agency, project numbers APVV-20-0015 and APVV-21-0289.

Halophilic bacteria - the „rising stars“ of next generation industrial biotechnologies

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Abstract: Due to their special characteristics, adaptation to life at high salt concentrations, and potential for a range of biotechnological applications halophilic bacteria are the rising stars of modern biotechnologies. They produce variety of products such as salt (and temperature) tolerant enzymes, osmoprotectants (ectoine, betaine), and biopolymers (polyhydroxyalkanoates - PHA). Multiple natural saline environments in Slovakia and Ukraine were analysed for the presence of halophilic bacteria. No true halophilic bacteria were detected in water sources with total dissolved salts (TDS) content lower than 10 g/L. Halophilic communities were detected in Slana voda natural spring (TDS 50 g/L) and in two salt brines from former salt mines (Solivar and Solotvino) with TDS more than 300 g/L. Cultivable bacterial communities in all three habitats were dominated by Proteobacteria - mainly by *Halomonas* spp. but multiple new species were isolated. Biochemical and genomic analyses confirmed that isolated strains are promising source of salt-tolerant hydrolases (amylases, cellulases, proteinases etc.) and high level of PHA production was detected in *Halomonas* spp. In the members of this genus the highest ability to decolorize synthetic azo dyes was observed. Our data indicate that natural salt springs could be an unique source of new species of halophilic bacteria with valuable properties.

Keywords: bacteria, extremophiles, biotechnology

Trehalose synthases fused with a maltokinase – an *in silico* analysis

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Abstract: Trehalose synthase (TS), a member of the subfamilies GH13_16 and GH13_33 of the α -amylase family GH13, catalyses the interconversion of maltose and trehalose. Some of the GH13_16 TSs may contain a maltokinase (MaK), suggesting their role in the 4-step metabolic pathway of glycogen biosynthesis recently revealed in some bacteria. Of total 5,933 GH13_16 members, 3,347 non-redundant TS sequences were selected and analysed for the presence of the eventual MaK domain succeeding the TS. A group of 1,425 enzymes containing the complete MaK fused to TS was collected; the MaK domains being compared with true MaK and analysed in detail. While most of the fused enzymes contain a standard MaK with conserved catalytic residues and a binding site for maltose, some contain just a MaK-like domain that is probably not active due to mutations in the MaK catalytic residues and/or in the binding site for maltose. Analysis of the linker region connecting MaK to TS suggests that the MaK domains in fused enzymes are likely to be longer than those found in true MaKs. The present bioinformatics analysis could thus help in studying the role the MaK and/or MaK-like domains may play in conjunction with GH13_16 TSs.

Keywords: CAZy database; GH13_16 subfamily; trehalose synthase; maltokinase; fused enzymes; bioinformatics

Detection of Xanthomonads on the commercially available seeds of *Brassica* species

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Abstract: During commercial seed production, vegetable seeds may become infected with various bacterial phytopathogens after systemic colonization of plants upon leaf infection. The species *Brassica oleracea* included many well-known crops such as cabbage, kale, kohlrabi and broccoli, grown and consumed worldwide. Black rot is one of the most important diseases that affect *B. oleracea* crops, reducing the quality of crops and causing great economic losses. This disease is caused by Gram-negative bacteria *Xanthomonas campestris* pv. *campestris* (Xcc). Moreover, other representatives of the genus *Xanthomonas* can incite leaf-spot disease. Thus, we were interested in quick detection of potentially presented bacterial pathogens on seed surface of four mentioned *Brassica* species. Bacteria cell suspension (eluate from seeds surface by TRIS-EDTA buffer cultivated on Nutrient agar) we used directly in PCR detection. We tested universal 16S rRNA primers as well as specific primers for identification of *X. campestris* pv. *campestris* (Xcc), *X. perforans* (Xp), *X. euvesicatoria* (Xe), *X. gardneri* (Xg) and *X. vesicatoria* (Xv). We confirmed the presence of bacterial microorganisms on the seed surface of all tested *Brassica* species using 16S rRNA primers. Among tested Xanthomonads, we found the presence of only *X. euvesicatoria* on seeds of kale, kohlrabi, broccoli as well as cabbage.

Keywords: *Brassica* sp., PCR, phytopathogenic bacteria, *Xanthomonas* sp.

Acknowledgement: The authors acknowledge support by the grant INTERREG 304011X035.

Essential oils containing caryophyllene and their antibacterial effects

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Abstract: Terpenes have antimicrobial, antioxidant, and other biological effects, which influence the use of many plants in traditional medicine, in the food and cosmetic industry. Plants produce terpenes that occur in essential oils produced in glandular secretory cells. A unique terpene is caryophyllene, which occurs in four structural forms such as α -humulene, β -caryophyllene, isocaryophyllene and caryophyllene oxide. The aim of this work was to characterize the antibacterial potential of selected essential oils containing caryophyllene against *Escherichia coli* CCM 3954, *Micrococcus luteus* DSM 1790 and *Staphylococcus aureus* CCM 4223 by microdilution and disk diffusion methods. The most significant effects were observed with oregano and clove oil, whose minimum inhibitory concentrations (MIC) for all tested bacteria were less than 1 μ l/ml. Oregano oil formed inhibition zones of 22.5-25.0 mm and clove oil 20.0-22.0 mm at a concentration of 128 μ l/ml. Lavender oil also had significant antimicrobial potential with MIC less than 1 to 4 μ l/ml and inhibition zones of 19.5-24.5 mm at a concentration of 128 μ l/ml, as well as clary sage oil with MIC less than 1 to 8 μ l/ml and inhibition zones of 15.5 – 20.0 mm. The most sensitive was the gram-positive bacterium *S. aureus* CCM 4223 with MIC less than 1 μ l/ml for all tested essential oils. Other bacteria were less sensitive. Among the tested pure substances, β -caryophyllene and α -humulene showed weak antimicrobial activity at MIC 512 μ l/ml, except for *S. aureus* CCM 4223, where the MIC of β -caryophyllene was 256 μ l/ml and α -humulene 32 μ l/ml. In the disk diffusion test, concentrated α -humulene formed inhibition zones 20.5-30.0 mm and β -caryophyllene zones were 21.5-26.0 mm in diameter. Gram-positive bacteria were the most sensitive to the effect of the pure substances. In our work, we confirmed the antibacterial effect of essential oils containing caryophyllene. Essential oils with β -caryophyllene as one component were more effective than pure substances.

Keywords: terpenes, β -caryophyllene, α -humulene, antibacterial activity, MIC, *Escherichia coli*, *Micrococcus luteus*, *Staphylococcus aureus*

Acknowledgement: The authors acknowledge support from APVV-20-0413

The expression level of the CysPC domain of mitochondrial calpain in W10BSmL white mutant compared to wild type *Euglena gracilis* strain Z.

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Abstract: Calpains (EC 3.4.22.17) are a family of calcium-activated cysteine proteases that participate in many cellular processes. Defects in the functionality of calpains cause various deficiencies in organisms. Currently, calpains are well-characterised in many animals and plants, but there is still poor information about their function in the protist taxon *Euglenida*. The group of photosynthetic euglenids belongs to the supergroup Excavata. These flagellates are often used as model organisms in transcriptomic research. The mitochondrion of *Euglena gracilis* is a single, large and reticulated organelle, a trait that is by no means unique among protists. Recently, the sequence of mitochondrial calpain was identified in the transcriptome of *E. gracilis* using in silico methods. Mitochondrial calpain consists of conservative CysPC and Calpain III domain. The main aim of this work was to detect and compare the gene expression level of mitochondrial calpain of the wild-type *E. gracilis* strain Z and its stable bleached mutant W10BSmL. We isolated total RNA from cell cultures grown for 24 h at light and a temperature of 23 °C. Further, complementary DNA was prepared by reverse transcription process, and 2 ng/μl cDNA was added to the reaction mix. Using qRT-PCR analysis, we amplified a segment of the CysPC domain of the mitochondrial calpain and *cox1* gene (one of the seven till now detected proteins coded by the mitochondrial genome of *E. gracilis*, which we used as a reference gene). The relative expression we interpreted according to the Livak method. We found that in the white mutant W10BSmL, the activity of the mitochondrial calpain gene significantly increased more than 2.5 times.

Keywords: CysPC domain, *Euglena gracilis*, mitochondrial calpain, qRT-PCR, W10BSmL mutant



Applied Informatics

Echo state network as polynomial approximator

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Abstract: Echo state network (ESNs) as a specific type of recurrent neural network (RNNs) has gained a lot of attention within the research community. It is probably the most prominent representative of so-called Reservoir Computing (RC) methods, where a “huge” randomly created and untrained reservoir serves as the source for trainable readout mechanism. Training of ESNs is much less computationally demanding, since unlike the more common fully trained RNNs, only a small part of ESN parameters is trained.

A lot of interest was devoted to the understanding of ESN's ability to achieve the state-of-the-art performance on some tasks and many interesting theoretical results are related to the study of the ESN's memory capacity, often ignoring nonlinearity of activation function. In this contribution, we study ESN as a polynomial approximator. We show that models with considerably simpler low-order polynomial activation functions can achieve the very same performance as regular ESNs, and then we suggest RC models with reservoir formed using polynomials and compare results with regular ESNs.

Keywords: Echo State Network, Reservoir Computing, Random Networks

Acknowledgment: This research was funded by KEGA 020UCM-4/2022.

Research and analysis of IT specifications of good practices in the area of artificial intelligence

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Abstract: This article is fulfilled within the framework of Erasmus+ project “The Future is in Applied Artificial Intelligence” (FAAI) and examines research of collecting IT specifications of good practices in Area of Artificial Intelligence (AAI). The article describes research conducted, the purpose of which is to find IT specifications of good practices in AI and describe their characteristics, like an area of implementation of the AI solution, the result of processing the data, the source of data, Data processing, and quality, what tools are used for processing data, and others. AAI application cases are reviewed and the technologies used to implement it, the specifics of the data, and the applications used are described. The analysis of the technologies thus described will give an idea of the preferred ones among them and give the picture of the so-called "good practices" in this field.

The research was done by looking at cases all over the world. The analysis of the data provides insight in several directions:

- Application area of ML/AI
- Type of machine learning problems in described good practices in Artificial Intelligence
- Type of models were developed within the projects
- What is the area of implementation of AI solution
- Used AI libraries (frameworks).
- Source of data
- Data characteristics
- Tools are used to store data
- What platform solution is used
- What type of storage is used

The research and analysis done provide a clear picture of the used IT specifications of good practices in AI. The obtained results will guide in what areas to organize the practical training in the preparation of specialists in the AAI. Also, this research would help future AI application developers.

Keywords: Artificial Intelligence, Applied Artificial Intelligence, Good Practices, Training, FAAI

Acknowledgments: This publication was published with the assistance of by Erasmus+ Project No. 2022-1-PL01-KA220-HED-000088359 entitled by "The Future is in Applied Artificial Intelligence" (FAAI) [4], which aims to join together HEIs and businesses and from National Scientific Programme "Security and Defence", adopted by RMS No. 731 of 21.10.2021 under Agreement No. D01-74/19.05.2022.

Research and analysis of different real cases, with use AAI

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Abstract: This article is fulfilled within the framework of Erasmus+ project “The Future is in Applied Artificial Intelligence” (FAAI) and examines the study of practical solutions implemented using applied artificial intelligence. The research was done by preparing an online survey. The purpose of the study is to find real working applications of applied artificial intelligence projects, describe their application in the relevant field, and record the name of the projects found to describe their activity. The study was done by looking at cases all over the world. The analysis of the data provides insight in several directions:

- in which countries are more of real cases of artificial intelligence solutions applied
- what is the distribution of realized cases - depending on whether the country is a member of the EU or not EU.
- In what category is the real case developed.
- whether the country of the real case works in collaboration with other countries or implements the real case only within the country of origin.

The resulting research and analysis provide a clear picture of the developed projects using artificial intelligence. The obtained results will guide in what areas to organize the practical training. Also, the research would help future AI application developers.

Keywords: Artificial Intelligence, Applied Artificial Intelligence, Good Practices, Training, FAAI

Acknowledgment: This publication was published with the assistance of by Erasmus+ Project No. 2022-1-PL01-KA220-HED-000088359 entitled by "The Future is in Applied Artificial Intelligence" (FAAI) [https://faai.ath.edu.pl], which aims to join together HEIs and businesses. The given work results are within the framework of the FAAI work package 2 entitled by "Good practices in the use of Artificial Intelligence and Machine Learning" and are presenting real cases that are offered for studying of applied AI. This publication was also supported and published with the assistance of the National Security and Defense Scientific Program, approved by RMS No. 731 of 21.10.2021 under contract No. D01-74/19.05.2022.

The principles of data mining and machine learning techniques with R

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Abstract: Data analytics has revolutionized the way businesses operate and make decisions. Gaining valuable insights from large amounts of data has opened endless possibilities in a variety of industries. Data analytics is finding applications in almost every industry. In this paper, we will discuss the real-world applications of data analytics and its profound impact on businesses and society. The paper explains selected data mining principles and machine learning techniques and emphasizes the importance of applied and multidimensional modeling in language R. We emphasize the detailed explanation of the selected techniques, while also providing real-world examples with data from different domains. The examples use the latest R language syntax with recognized robust, extended, and up-to-date packages.

In addition, we focus on the concept of spatial analysis, allowing to build user's own maps through geo-referenced data and some basic statistical techniques. The other part of the paper covers GeoXp, an R package implementing interactive graphics for exploratory spatial data analysis. To illustrate the use of these exploratory techniques based on linking a statistical graph and a map, we use a dataset related to Slovak public schools of the cvtivr research library. In addition to basic graphs such as boxplots, histograms, or simple scatter plots, GeoXp also links maps with Moran scatter plots, variogram clouds, Lorenz curves, and other graphical tools. To make the best use of the multidimensionality of the data, we have used dimension reduction techniques such as principal component analysis and cluster analysis, the results of which are also linked to the map.

Keywords: data analysis, data mining, machine learning techniques, language R, spatial analysis, graphs

Acknowledgment: The author acknowledges support from KEGA 020UCM-4/2022.

Applying a dynamic control system model to optimize and test time series forecasting using deep learning

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Abstract: Modern systems for the control of complex processes in various areas of life actively use recurrent neural networks (RNN). A neural network with long-term memory (LSTM) allows the prediction of the subsequent values of a time series. The proposed paper provides a universal model of a dynamic system in SIMULINK of the MATLAB environment. Tuning the model parameters ensures the generation of a training sequence of values for the LSTM, the optimization of the RNN structure, and its testing. The generation of the training sequence is synchronized with the time step of the RNN input sequence.

Keywords: neural networks, Simulink, MATLAB, optimization

Acknowledgment: The work was funded by the grant KEGA 012UCM-4/2021 Modern technologies and innovations in network security education.

Possibilities of using heart rate variability data to control serious games

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Abstract: Serious games have become increasingly important in recent years due to their expanded relevance and potential for innovative technological advancements, such as the monitoring of physiological variables. These opportunities offer valuable insights into controlling and monitoring games, specifically by utilizing data obtained from the unique physiological impulses of each player. This paper aims to explore the integration of devices that enable the control of educational games through synchronously monitoring data on the player's heart rate variability (HRV). HRV-based physiological responses can be acquired using specialized hardware, providing objectively obtained data for immediate analysis, evaluation, and interactive application control. This approach offers the potential to prospectively understand player activity and behavior, leading to advancements in personalized adaptive systems, game design, and the development of specialized devices for human-computer interaction. Implementation of HRV technology into serious games may have significant implications for both the gaming industry and future scientific research.

Keywords: serious games, development, HRV, data analysis

Acknowledgement: The work was funded by the grant VEGA 2/0070/21 Nízko-dimenzionálne materiály – manipulácia, funkcionalizácia a bioaplikácie: LOW-D-MATTER.

Assessment of DDoS Attack Simulation Tools

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Abstract: The paper focuses on simulations of DDoS attacks in network simulators and a comparison of simulation environments. Large-scale DDoS attacks on UDP and ICMP protocols on IPv4 and IPv6 networks were investigated using four network simulators: NS3, Cisco Packet Tracer, OMNeT++, and NetSim.

The article provides an overview of the IPv4 and IPv6 Internet protocols and their structure, as well as different types of DDoS attacks and their characteristics. It also introduces four main network simulators and their capabilities to model DDoS attacks. Using practical experiments, DDoS attacks on a server have been simulated. Two simulation scenarios were performed. The first scenario measured the difference between UDP and ICMP packets received and sent by legitimate clients on the server, with 30 attacking zombies sending packets to the server. The best-performing simulator was OMNeT++, where both types of attacks were successfully simulated on both IP protocols. The NetSim simulator lacked IPv6 support, and the ICMP attack was only possible using the emulator. The NS3 simulator allowed only for a UDP attack on the IPv4 protocol, with different data processing. In the second scenario, the server response time to an ICMP packet from a legitimate client was measured, while zombies attacked the network at different packet-sending intervals. This simulation was only successfully performed on the OMNeT++ simulator, with server response times per ICMP packet being larger and more frequent than in the perfect environment.

The results obtained indicate that the different simulators achieved varying levels of accuracy and reliability in modeling DDoS attacks and their impact on network performance. In particular, the OMNeT++ and NetSim simulators stood out, achieving the best results when simulating both types of attack on both versions of the Internet Protocol. The NS3 simulator demonstrated good performance in simulating a UDP attack on IPv4, but its support for the simulation of IPv6 and ICMP attacks was limited. Cisco Packet Tracer is not adapted to simulations with large topologies and large numbers of devices and is not a suitable tool for simulating DDoS attacks. The paper provides guidance in selecting the most appropriate simulator for DDoS attacks and offers the possibility of further studies in this area.

Keywords: DDoS attacks, Simulation, Analysis, Comparative study

Acknowledgment: The work was funded by the grant KEGA 012UCM-4/2021 Modern technologies and innovations in network security education.

Development of algorithmic and critical thinking in the context of programming using instructive and engaging explainer animated videos

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Abstract: In Slovakia, we have been observing a long-term decline in teaching technical and natural sciences quality across all levels of schools from lower through upper secondary, including specific and professional subjects such as algorithmization and programming. It is also a societal need, as thousands of computer scientists are currently missing to fill specialized positions in practice. We perceive knowledge of the basics of programming and algorithmic thinking not only as digital competences but also as a tool for the development of logical thinking. Algorithmic thinking contributes significantly to several key competencies such as problem-solving, computer literacy, mathematical literacy and logical thinking. We try to support these by creating and using instructional videos and animated videos with elements typical of explainer animated videos, which are also successfully used in marketing.

Keywords: instruction video, explainer animated video, algorithmization, programming, linked list

Acknowledgement: The paper was funded by the grant KEGA 017UCM-4/2022 Development of an interactive e-course using “SMART” technologies for the development of algorithmic thinking and programming skills.

Neural networks in natural sciences

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Abstract: Artificial neural networks (ANNs) have emerged as powerful tools for addressing complex problems in various fields, including the natural sciences. This contribution involves an exploration of the applications of artificial neural networks, specifically focusing on their use in both regression and classification tasks. We place particular emphasis on utilizing the autoencoder model within the context of the anomaly detection in natural sciences.

The autoencoder, a type of unsupervised learning model, has gained significant attention due to its ability to catch meaningful representations of input data. Its architecture comprises an encoder, which compresses the input data into a lower-dimensional latent space, and a decoder, which reconstructs the original input from the encoded representation. This unique characteristic of the autoencoder makes it well-suited for extracting valuable features from high-dimensional scientific datasets. We will present some applications of the above-mentioned models in the natural sciences and highlight the advantages, such as their ability to handle noisy and incomplete data.

Keywords: artificial neural networks, regression, classification, autoencoder

RL-Toolkit: Design and implementation of a set of tools for reinforcement learning in robotics

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Abstract: This paper presents a novel toolkit for self-learning of robots in simulated environments, with a focus on maximizing task performance scores. The proposed method utilizes an artificial neural network to transform sensor measurements into an action vector, i.e., the movements of the robot's motors, employing reinforcement learning principles to maximize the quality of state transitions resulting from performed actions. The Reverb database server is employed for storing interaction data obtained during simulations. Experimental results demonstrate a significant improvement of 9.38% over the published results of the original algorithms. The design of the RL-Toolkit comprises a database server, a Weights & Biases monitoring tool, and support for three popular simulation environments (Gymnasium, DeepMind Control Suite, and PyBullet). Furthermore, an architecture design is provided for applying the RL-Toolkit to real-world robots, showcasing its potential for practical implementation.

Keywords: soft actor-critical model, deep neural network, Gymnasium, robotics, Q-value, quantile regression, Docker

Acknowledgment: The work was funded by Erasmus+ project FAAI: The Future is in Applied Artificial Intelligence - 2022-1-PL01-KA220-HED-000088359.

ARphymedes and ARphymedes plus projects: modern ways of learning physics with augmented reality

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Abstract: ARphymedes, short for "Augmented Reality Physics Made for Students", recalls the name of one of the most famous physicists in history: Archimedes. The goal of the project is to enable children to explore and realize their dreams with the help of "Augmented Reality" (AR). With this aim, a consortium of physics teachers, engineers, historians, and IT professionals design a modern and exciting set of textbooks and augmented reality applications for students and teachers. This tool will put the student on the path of exploring physics with the possibility to interactively test and experiment right from their desk. In addition, we are also working on a project Arphymedes Plus that allows using the potential of the ARphymedes project specifically for children with disabilities.

Keywords: augmented reality, interactive experiments, learning physics, history of physics, students with special needs

Acknowledgement: This work is supported by the Erasmus plus Programme of the European Union Arphymedes grant agreement number 2020-1-SK01-KA201-078391 and Arphymedes plus grant agreement number 2020-1-SK01-KA226-SCH-094415.

Comparison of semantic similarity detection algorithms in the evaluation of automated open-ended questions in the Slovak language

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Abstract: One of the problems in dealing with the evaluation of automated short answer testing (ASAG) is in the case of open-ended questions. The syntactic complexity and semantics within a given natural language processing cause various problems in the relevance of the results during evaluation. Different kinds of applications use different ways of interpreting the information entered. In our context, applications such as LMS Moodle - quiz, Socrative, Google Forms, and MS Teams - test portal are often used. However, there are also other approaches to evaluating the context of the input information. This paper presents a comparison of algorithms focused on the semantic similarity of information in the evaluation of final assessments in digital form. Whichever algorithm we analyzed, the human approach plays an irreplaceable role. While automated evaluation gives us fast results, without manual back-checking the correctness of the evaluation would be more than questionable.

Keywords: Sentence Transformer, SBERT, Semantic similarity detection, short answers

Acknowledgment: This research was funded by the grant KEGA 020UCM-4/2022 and by the grant KEGA 017UCM-4/2022 Development of an interactive e-course using "SMART" technologies for the development of algorithmic thinking and programming skills.

The ethics of artificial intelligence: Issues and challenges

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Abstract: Artificial intelligence (AI) is transforming various aspects of human society, such as economy, health, education, security, and entertainment. However, along with the benefits and opportunities, AI also poses significant ethical challenges and risks, such as privacy violations, discrimination, bias, lack of transparency, accountability, and human dignity. These challenges and risks may undermine the trust and acceptance of AI systems by the public and affect their social and legal implications. Therefore, it is essential to ensure that AI is developed and used in an ethical and responsible manner that respects human rights and values. This paper aims to provide a comprehensive and critical overview of the main ethical issues and challenges arising from the development and deployment of AI systems. It also discusses some of the existing frameworks and principles for AI ethics, such as the ones proposed by the European Commission, the IEEE, and the OECD. However, it also points out the gaps and limitations that need to be addressed, such as the lack of enforceability, diversity, and stakeholder participation. Furthermore, it proposes some recommendations and best practices for ensuring that AI is aligned with human values and promotes social good, including the need for interdisciplinary collaboration among various stakeholders, such as researchers and practitioners.

Keywords: AI ethics, AI accountability, AI transparency, AI bias, AI regulation, AI safety

Acknowledgement: This research was funded by the Cultural and Educational Grant Agency MŠVVaŠ SR, grant number KEGA 020UCM-4/2022, and by Erasmus+ project FAAI: The Future is in Applied Artificial Intelligence - 2022-1-PL01-KA220-HED-000088359, work package WP4

Implementation of the algorithms for finding the shortest path using LEGO Mindstorms

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Abstract: The utilization of the LEGO Mindstorms platform is on the rise within technically oriented universities. This popular platform is actively integrated into higher education to develop logical thinking, teach fundamentals of algorithms and programming, provide robotics instruction, and enable discovery and experience in mechanics, dynamics, construction, sensors, electric motors, and control systems. This platform positively affects spatial imagination, combination skills, teamwork and communication, and the ability to plan and abstract or think analytically. Many researchers in this area have confirmed that the use of LEGO Mindstorms contributes to increased activity in learning programming.

This paper is focused on the application of algorithms for path planning and finding the shortest path using Lego Mindstorms. It describes and analyzes the A star algorithm, for which we have chosen Manhattan, Chebyshev and Euclidean distance heuristics and the BFS algorithm, which are used in path planning and solving navigation problems. As a criterion for comparing individual algorithms, we chose the total path calculation time and path length.

Keywords: LEGO Mindstorms, A star algorithm, BFS algorithm, path planning, Java, Eclipse

Acknowledgment: The work was funded by the grant KEGA 012UCM-4/2021 Modern technologies and innovations in network security education.

Virtualization in the preparation of experts for advanced solutions of network security

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Abstract: Nowadays, network attacks are a constant threat that every organization connected to the Internet has to deal with. This is precisely why experts in network security solutions are in high demand in the job market. Universities also participate in the preparation of such experts in the form of face-to-face or distance education. Virtualization technologies are intensively used in both forms. The most commonly used technologies are Proxmox VE and VirtualBox.

In the paper, both of these technologies were compared from the point of view of lecturers and attendees of the educational course Advanced network security solutions. The valued advantage of Proxmox from the lecturer's point of view was that it eliminated the problem of locating any problem that the attendee got stuck on. The lecturer did not have to search whether the problem is in the operating system on the virtual machine, or at the level of virtualization, or at the level of the operating system that runs on the attendee's computer. Thanks to the fact that the lecturer had administrative access to the PVE, he could work directly with the attendee's VMs and debug any problems. Then, using a simple video conference and sharing the application window, he could show and explain to the attendee where the problem is and how to solve it. Attendees appreciated Proxmox for the possibility of immediate work with VM without the need to install SW, since a browser is enough to work with Proxmox. The article summarizes the advantages and disadvantages of the virtualization environments used by lecturers and attendees.

Keywords: network security, virtualization, Proxmox, Virtual Box

Acknowledgment: The work was funded by the grant KEGA 012UCM-4/2021 Modern technologies and innovations in network security education.



Young Scientists

Determination of anthropogenic contamination in soil profiles in the geologically anomalous landscape of northwestern Bohemia

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Abstract: The area of northwestern Bohemia is known for great geological diversity and also for its changes caused by extensive anthropogenic activities in the past. Agricultural land in that area has elevated concentrations of some risk elements for (e.g. arsenic or beryllium), however, it is not clear if these have resulted from anthropogenic contamination or from natural anomalies in the bedrock. Contamination of NW Bohemia can come from both ore mining and processing and coal mining and combustion. In the case of coal mining and utilization, contamination by atmospheric fallout (As, Cd, Sb) regardless of the bedrock, while contamination from ore mining and processing (As, Sb) can be expected to have smaller spatial impact around historical mines and smelters. Both should increase upward in soil profiles. So far, several dozen profiles have been sampled in the Teplice region and in the Ore Mountains and the reference locality NW of Lovosice. The analytical methods in this work include acid extractions and analysis by ICP-MS, as well as total analyses by XRF. The aim of this work is to distinguish natural contamination from the bedrock and the consequences of anthropogenic activities.

Keywords: soil contamination, NW Bohemia, Bedrock, ICP-MS, XRF

Plant RNA virus as a tool for the expression of foreign polypeptides

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Abstract: Expression vectors based on plant viral genomes provide a promising way of rapid, cost-effective and scalable production of recombinant proteins in plants. Among numerous genera of plant viruses used for this purpose, potyviruses (genus *Potyviridae*) offer several advantages, such as polyprotein expression strategy, or a broad host range. In our work, the expression vector pAD-agro based on plum pox virus (PPV) genome was successfully applied for the expression of different heterologous polypeptides in *Nicotiana benthamiana* plants including two plant viral capsid proteins, bacterial heat-shock protein, a fragment of influenza A virus hemagglutinin or SARS-CoV-2 nucleoprotein (N) and its fragments. Particular proteins differed in their accumulation rate, tissue localization, stability and solubility. The highest accumulation was observed in case of the N-terminal half of N SARS-CoV-2 that was successfully purified from infected leaves by immobilized metal affinity chromatography in presence of 6M guanidine hydrochloride. In contrast, the C-terminal half of N SARS-CoV-2 showed significant signs of proteolytic degradation *in planta*. Interestingly, the fusion of a native *N. benthamiana* extensin secretory signal to the N-terminus of this fragment improved its stability, indicating that targeting proteins of interest to the apoplast may help to increase their accumulation rate.

Keywords: viral vector, transient expression, potyvirus, plum pox virus, agroinfection

Acknowledgement: This work was supported by the grant APVV-20-0015 and VEGA 2/0003/22.

Detection and molecular characterization of viroids infecting grapevine (*Vitis vinifera* L.) in Slovakia

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Abstract: Grapevine (*Vitis vinifera* L.) represents an important agricultural crop with historical tradition of cultivation and world-wide distribution. However, grapevine is also a known host of several yield-threatening plant viruses and viroids. Viroids are characterized by their relatively simple composition consisting only of naked single-stranded circular RNA molecule, a few hundred nucleotides in length, without protein-coding properties. These peculiar plant pathogens, basically infectious RNAs, are thus categorized as subviral entities and potentially even the smallest parasites in nature. Seven distinct viroid species were identified to be able to infect grapevine, but only three occur frequently within central European region, i.e. *hop stunt viroid* (HSVd); *grapevine yellow speckle viroid 1* and *2* (GYSVd-1 and GYSVd-2). In this work, we report the detection of two viroid species (HSVd and GYSVd-1) in our environmental samples via high-throughput as well as standard Sanger sequencing. Despite of their studied omnipresence in neighbouring countries, these findings represent the beginning of initial country-wide survey regarding the prevalence of grapevine viroids in Slovakia. Finally, we perform further molecular analyses of Slovak viroid isolates based on their predicted RNA secondary structures aiming to better understand the mechanism of their host-specific adaptation and evolution.

Keywords: high-throughput sequencing, grapevine, viroid, secondary RNA structure, HSVd, GYSVd-1

Acknowledgment: Work is supported by the grants APVV-22-0067 and FPPV-33-2023.

***Alnus glutinosa* and soil microbial community response to HCH contamination**

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Abstract: While the pesticide hexachlorocyclohexane (HCH) and its isomers have long been banned, their presence in the environment is still reported worldwide. In this exterior study, our objective was to determine the bioaccumulation potential of α , β and δ -HCH isomers by Alder saplings (*Alnus glutinosa*). Each HCH isomer was mixed separately with soil to achieve a final concentration of 50 mg/kg. All variants, including a control without HCH, were set in triplicate and had instant access to water for three months. Subsequently, HCH levels were assessed in soil and seedling sections (root, trunk, branches, leaves) by gas chromatography-mass spectrometry, while amplicon 16S rRNA sequencing was used to study the rhizosphere and soil microbial community. Highest HCH isomer concentrations were detected in roots, with a decreasing trend toward branches and leaves. The δ -HCH isomer was taken up in highest quantities (roots - 14.7 $\mu\text{g/g}$, trunk - 7.2 $\mu\text{g/g}$, branches - 1.53 $\mu\text{g/g}$, leaves - 1.88 $\mu\text{g/g}$), with α -HCH and β -HCH recorded at much lower concentrations. Interestingly, high concentrations of α -HCH were also detected in the β -HCH polluted soil. Phytohormone analysis indicated that *A. glutinosa* reacted to HCH contamination through changes in cytokinin, jasmonate, abscisate and gibberellin content. With some exceptions, rhizosphere microbial population abundance was similar in all HCH isomer samples, e.g. the common soil bacterium *Pseudomonas* spp. decreased in all HCH-amended samples, while *Tomentella* was dominant in β -HCH and control rhizosphere samples and lowest in δ -HCH samples. Further studies will be undertaken to elucidate why δ -HCH was most easily bioaccumulated.

Keywords: Alder, *Alnus glutinosa*, biodegradation, hexachlorocyclohexane, phytoaccumulation, phytoremediation

A new electrochemical method for the determination of carnosine in nutritional supplements

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Abstract: Carnosine is a dipeptide composed of β -alanine and L-histidine. It has antioxidant, pH buffering, chelation, and anti-glycation effects. Food supplements containing carnosine are currently being produced for these effects. However, no one controls the amount of carnosine in these supplements yet. For that we have developed a fast and financially more affordable electrochemical method, using the differential pulse voltametric technique, which can reliably determine carnosine concentrations in supplements. During the development of the method, we optimized the choice of the pH of the buffer solution, with the aim to obtain the best signal and scale down LOD. Experiments were performed using a potentiostat (Autolab AUT84456), a boron-doped carbon electrode, a platinum auxiliary electrode and an Ag/AgCl reference electrode. After optimization, we created a calibration dependence in which we determined the linear range (0.05mM to 0.75mM), sensitivity as well as LOD (0.082mM) and LOQ (0.250mM) of the given method. The influence of the matrix on the carnosine analytical signal was investigated. After optimising the given parameters, determination of carnosine in nutritional supplement sample was performed. The determined concentration of carnosine in nutritional supplements coincided with the declared concentration of the manufacturers.

Keywords: differential pulse voltammetry; nutritional supplements; carnosine

Acknowledgement: This study was realized with support of project KEGA 025UCM-4-2021.

Zero-field splitting in tetracoordinate Co(II) complexes containing heterocyclic aromatic ligands

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Abstract: Tetracoordination is a frequent structural motif among transition-metal complexes. A special attention is paid to the tetracoordinate Co(II) complexes since a lot of them show SMR. A series of tetracoordinate mononuclear Co(II) complexes $[\text{Co}(\text{L}^1)_2(\text{X})_2]$ (**1-3**) and $[\text{Co}(\text{L}^2)_2(\text{X})_2]$ (**4-6**) {where $\text{L}^1 = 2\text{-amino-1-methylbenzimidazole}$; $\text{L}^2 = 4\text{-methylquinoline}$; $\text{X} = \text{Cl, Br, I}$ } have been synthesized and studied in detail. Compounds were characterized by spectroscopic methods along with their molecule structure determined by the single-crystal X-ray diffraction. All complexes have been investigated in the static magnetic field $B_{\text{dc}} = 0.1$ T using SQUID magnetometry. DC magnetic data were fitted by a spin Hamiltonian model appropriate to a zero-field splitting system. The axial zero-field splitting parameters D ranged as -14.44 (1), -13.05 (2), -7.50 (3), -6.76 (4), $+7.19$ (5), -5.58 (6) cm^{-1} .

Keywords: cobalt(II) complex, paramagnetism, zero-field splitting

The effects of different tree species on soil properties and soil development

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Abstract: Forest reclamation is a very important issue of environmental studies, especially when considering human-affected sites as in coal mining areas. Depending on which tree species was used for artificial afforestation, the recovery of the affected site can take different development paths and result in very different outcomes in terms of the quality of the final biotope. Trees have both direct and indirect effects on soil properties and development. Also, the soil or substrate properties play a crucial role in the stability and development of the ultimate ecosystem likeness. Spoil heaps left after coal mining, especially spoil heaps artificially reforested with several different tree species, can serve as very valuable model sites for researching ecosystem development. Our research took place in the Lusatian mining area of Domsdorf I, where such reforested spoil heaps exist. We measured the leaf nitrogen balance index of trees growing on the spoil heaps: pine (*Pinus sylvestris*), birch (*Betula pendula*), red oak (*Quercus rubra*), sessile oak (*Quercus petraea*), lime (*Tilia cordata*), larch (*Larix decidua*), and alder (*Alnus glutinosa*), and performed phospholipid acid analysis, pH measurement, measurement of nitrate content in the soil under each tree species, and measurement of mesofauna and macrofauna abundance counted from the ground beneath the trees. The results of these analyses are, in some cases, unexpected for the respective afforested sites – most notably in case of the soil fauna which could potentially act as ecological engineers. When taking into account these puzzling results of soil fauna abundances, we can explain other aforementioned measured markers and support previously published works which show the importance of soil fauna-tree species (and their mutualistic symbionts) interactions.

Keywords: ecosystem development, reclamation, coal mining spoil heaps, tree species effect, soil fauna, soil properties

Drug sorption on miscanthus biochar prepared under different conditions

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Abstract: The drug concentration in environmental is slowly increasing because of higher using of pharmaceuticals and their insufficient ability to remove in conventional wastewater treatment plants. Some institutions are aware of this issue and are looking for other methods of wastewater treatment. One of the promising ways is using biochar, which is product of modern way of waste transformation - pyrolysis. Tested biochar was produced from second generation energy crops *Miscanthus x giganteus*, which can produce huge amount of biomass also in marginal or contaminated soil. Biomass was pyrolyzed under two temperatures 360 °C (M3) and 500 °C (M5). The tested drugs were atenolol (AT), sulfamethoxazole (SMX) and 17- α -ethynylestradiol (EE2). Both tested chars were able to prove ability of high absorption capacity. The removal was more than 80 % after 4h for AT and EE2. Tested Langmuir and Freundlich adsorption models described sorption mechanism in the case of AT for both biochar, SMX only for M3. Sorption from mixture solution was affected by competitive sorption on active sites. The inter-drug exclusions were observing. In the case of real wastewater, the sorption mechanism was influenced by water properties. But even so, the drugs removal efficiency was more than 60 %.

Keywords: sulfamethoxazole, atenolol, 17- α -ethynylestradiol, sorption, biochar, *Miscanthus*

Magnetoactive complexes containing bioactive ligands. A theoretical study

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Abstract: Transition metal complexes represent extremely variable structures, which is reflected in their diverse physico-chemical properties modulated both by the central atom and by ligands. This diversity is constantly increasing, as the unique contributions that transition metals bring to the overall structure of metal complexes depend on the various coordination numbers, geometries, redox potentials, as well as kinetic and thermodynamic characteristics. Many of them may also contain biologically active ligands. Thus, for such systems a variety of biological interactions can be expected. Specifically, interactions of complexes with DNA can arise due to different type of intermolecular contacts (covalent and/or non-covalent in nature). In addition, most transition metals contain unpaired electrons, which means that their complexes can also exhibit a wide variety of useful magnetic properties. So, it can be assumed that the potential of metal complexes as therapeutic agents with associated molecular magnetism may be one aspect of their utility. We therefore decided to examine a series of M(II) complexes (M = Fe, Co, Ni, Cu) that contains N-donor (3-(pyrimidin-2-yl)-1,2,4-oxadiazole; N,N-diphenylacenaphthylene-1,2-diimine) and N,O-donor (various Schiff bases) ligands using high-quality quantum-chemical calculations. Designed complexes were utilized in conjunction with modern multiscale and composite DFT (QMMM, r²SCAN-3c) and ab initio methods to probe structural, spectral and magnetic properties of complex-DNA systems.

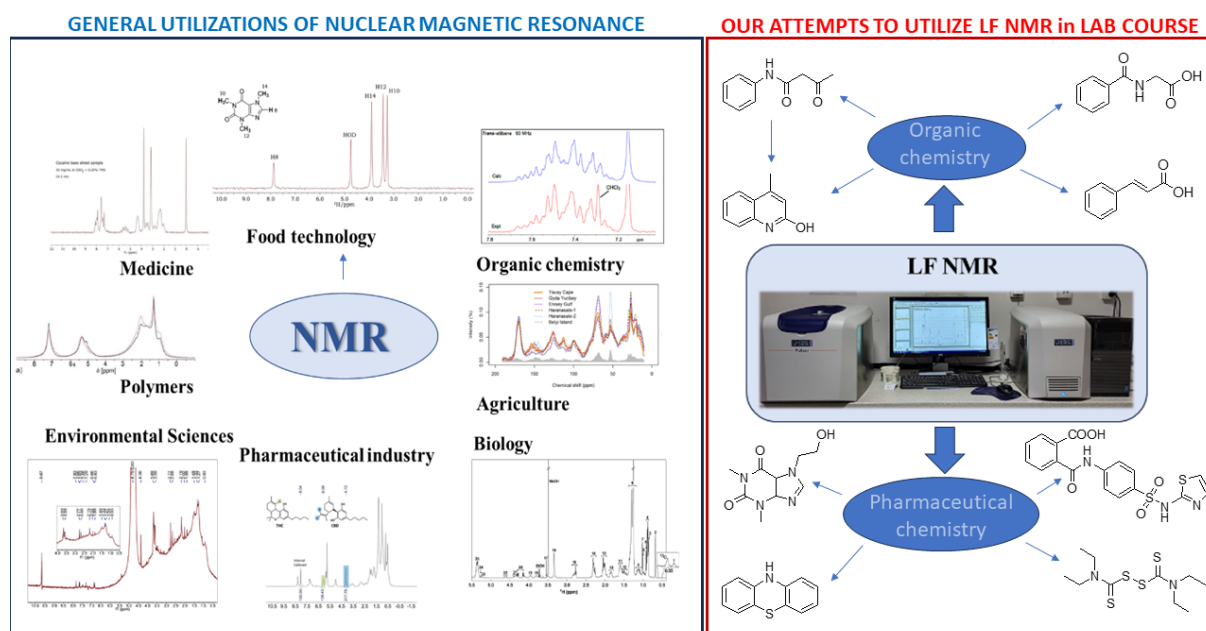
Keywords: metal complexes, DNA, molecular magnetism, multiscale methods

Benefits and use of LF NMR spectrometry in academic field and didactics

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Abstract: Research summarizes the advantage and use of the LF (low-field) NMR spectroscopy performed on a benchtop-type instrument (Oxford Pulsar, 60 MHz), compares the novel technique with traditional HF (high-field) nuclear magnetic resonance. Beyond the main benefits of LF NMR including economical-friendliness, smaller dimensions, easier maintenance and operation. LF-NMR offers easy and fast data acquisition, which is in behalf of general laboratory courses as an available spectral method. In our ongoing attempts to utilize LF NMR technique in a field of organic chemistry and synthesis, finally we have finally implemented the benchtop-type instrument as a part of laboratory course of pharmaceutical chemistry. Applying the particular spectral method in a course based on synthesis of drugs and pharmaceuticals, the combination of two fields of chemistry – the organic and analytical were uploaded in one leading to improvements from a point of view of quality and level of knowledge and experience gained during the academic study.



Keywords: benchtop NMR, high field NMR spectroscopy, organic chemistry, student laboratories

Acknowledgement: Financial supports from the Slovak Ministry of Education, Science, Research and Sport under the contract no. VEGA 1/0086/21 and VEGA 2/0055/21. The work was also financially supported by a grant of University of SS Cyril and Methodius with the project number UCM FPV05-2023.

Unraveling meiotic genes in euglenoid flagellates: Shedding light on protist evolutionary patterns

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Abstract: The evolution of sexual reproduction is intimately intertwined with the emergence of eukaryotes, with protists serving as the earliest actors in this evolutionary narrative. Among the diverse group of protists, euglenoid flagellates have garnered significant interest due to their unique gene expression regulation and evolutionary trajectory. The presence of meiotic genes within an organism's genome is a key prerequisite for sexual reproduction. In this study, we conducted in-silico analyses and initial in-vitro experiments to investigate the presence of essential meiotic genes in *E. gracilis*, a representative euglenoid flagellate. Our findings reveal that 8 out of the 9 essential meiotic genes have been identified in the genome and transcriptome of *E. gracilis*, with only one, SPO11, yet to be identified. Furthermore, phylogenetic analysis validates these preliminary results which holds great promise offering a fertile ground for further in-vitro experiments that may shed light on the origin and evolution of protists. This research contributes to our understanding of the fundamental processes underlying the emergence of sexual reproduction and provides a platform for future investigations into the intriguing world of protist evolution.

Keywords: *Euglena gracilis*, meiosis, gene expression

Identification and determination of *N*-Nitrosodimethylamine (NDMA) and *N*-Nitrosodiethylamine (NDEA) in losartan by GC-MS

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Abstract: Nitrosamines are classified by the ICH M7(R1) Guideline as Class-1 impurities and as "known mutagenic carcinogens", originating from organic synthesis and manufacturing process. The synthesis of drug substances involves use of reagents, chemicals, solvents and catalysts as potentially source of impurities. In Sartan substances, nitrosamines are formed by reaction of solvent impurities with nitrite ions in the acidic conditions. European Pharmacopoeia (Ph. Eur.) method for determination of selected nitrosamines (NDEA and NDMA) in losartan substances was modified with respect to dichloromethane extraction and validated for accuracy, precision, specificity, LOQ, LOD and linearity. Results met acceptance criteria and can be used for routine quality control of Losartan substance. Gas chromatograph SCION 456-GC coupled with the EVOQ GC-TQ with electron ionization and selected ion monitoring (SIM) mode was used in this study. Results confirmed presence selected determined nitrosamines in tested batches of losartan base.

Keywords: nitrosamines, active pharmaceutical ingredient, GC-MS, pharmaceutical substance

Repeated-batch Production of PHB by *Cupriavidus necator*

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Abstract: *Cupriavidus necator* bacteria are typical producers of polyhydroxybutyrate (PHB), which is the main representative of the polyhydroxyalkanoates (PHAs). The aim of this study was to evaluate selected fermentation conditions affecting the growth of the *C. necator* biomass as well as the intracellularly accumulation of PHB by repeated-batch production. PHA accumulation by *C. necator* occurs most frequently in response to environmental stress conditions. Therefore, a two-stage cultivation consisting of cultivation in propagation medium aimed at maximizing biomass production and subsequent cultivation in production medium aimed at maximizing PHA production appears to be the most appropriate method. The repeated-batch fermentations were carried out in ten cycles in a bioreactor, obtaining a dry biomass yield ~6.4 g/L and a PHB yield determined by GC ~59.1 %, averaged over each cycle. This suggests the potential of *C. necator* biomass utilization in multiple cycles without the need for always inoculation of bacteria and reducing the cost of PHB production.

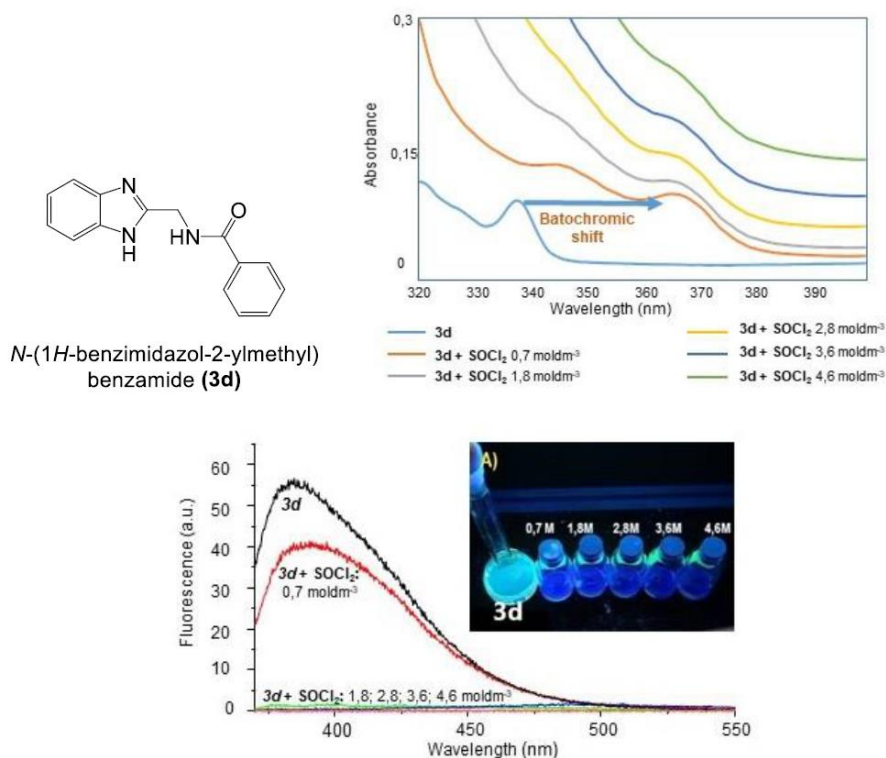
Keywords: *Cupriavidus necator*, PHB, repeated-batch cultivation, production

Analytical detection of substances with potential to damage environment and human health by benzimidazole-based fluorescent chemosensor

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Abstract: Benzimidazole and its derivatives are regarded as an important heterocyclic motif that exhibits a wide range of applications as benzimidazole derivatives are biologically active compounds. Synthesis of benzimidazole derivatives as potential chemosensor for readily reactive hazardous organic particles such as thionyl chloride (SOCl_2) and phosphoryl chloride (POCl_3) is presented. We have been able to prepare and identify target *N*-(1*H*-benzimidazol-2-ylmethyl)benzamide (**3d**) in acceptable yield and purity. It is essential to characterize synthesized products before sensing and changes in the chemical structure upon sensing. Changes in the structure and physico-chemical properties were observed by spectroscopic methods, including ^1H NMR, IR, UV-Vis, and fluorescence spectroscopy.



Keywords: chemosensor, fluorescence, UV-Vis, phosphoryl chloride, thionyl chloride

Acknowledgement: The financial support of the Slovak Scientific Grant Agency VEGA No. 1/0086/21 and VEGA No.2/0055/21 and the young scientists support of Faculty of Natural Sciences of University of Ss. Cyril and Methodius in Trnava with the contract number FPV-05-2023 is gratefully acknowledged.

The DNA markers and periopathogenic bacteria associated with periodontitis

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Abstract: Periodontitis is a multifactorial disease associated with the presence of molecular-biological factors, such as risky DNA polymorphisms as well as gram-negative pathogenic bacteria. Both factors participate in the development and progression of inflammatory processes in the gingival tissue.

The dysbiosis of the oral microbiome and long-term exposure to periopathogens (*Porphyromonas gingivalis*, *Tannerella forsythia*, and *Aggregatibacter actinomycetemcomitans*) represent the primary causes of chronic inflammation. Currently, several studies describe the association of selected DNA polymorphisms with the development of periodontitis (e.g. the DNA polymorphisms in *IL1A* and *IL1B*, *IL1RN*, and *TNF* genes), and have a strong pro-inflammatory activity leading to a higher risk of periodontitis. The DNA polymorphism in the *TNF* gene is associated with aggressive periodontitis and peri-implantitis and could participate in the process of bone loss. The presence of the *04 allele in the *HLA-DRB1* gene is considered a risk factor for bone resorption.

In addition to the routine clinical diagnostics of periodontitis, the extension of the spectrum of diagnostic DNA markers and bacteria, including those that are parallelly associated with the occurrence of periodontitis and complex systemic diseases (such as psoriasis, rheumatoid arthritis or cardiovascular diseases), could be important in the overall and personalized treatment of the patient.

Keywords: periodontitis, interleukins, HLA system, periopathogenic bacteria

Characterization of biomass wastes and its possibility of agriculture utilization due to biochar production by pyrolysis

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Abstract: The utilization of biomass for biochar production seems to be an efficient and environmentally friendly way of biomass treating. The pyrolysis is a cleaner and more sustainable process compared to direct combustion. Produced biochar can be utilized as soil amendment, because it can improve soil properties by many ways. Biochar is produced from various biomass by pyrolysis. Depending on the selected raw biomass, its composition and properties change. Lot of published works deals with commodities, which are not in current disposal in Central Europe, like bamboo or rice. In this work, twelve different local biomass wastes have been characterized in order to find out their suitability of biochar production which can be further used as a soil amendment. These wastes are generated in the production of vegetable oil, wine, beer, sugar, flour and of wood processing. The macro and micro nutrients were determined, simultaneously with the contents of toxic elements that disable the use of biochar in agriculture. The behaviour of biomass during the pyrolysis was simulated by thermogravimetric analysis. After evaluating all the results, the sample „Extracted rapeseed meal“ was assessed as the most suitable material for biochar production due to high nutrients content and suitable thermal stability.

Keywords: biomass waste, biochar, soil amendment

A reversible temperature induced spin crossover in Fe(III) complex

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Abstract: Substituted salicylaldehyde combined with the asymmetric (propyl/ethyl) triamine gave the pentadentate Schiff base $L^5 = 3\text{-EtO-salpet}$ which after complexation with Fe(III) center in presence of selenocyanate forms the target complex $[\text{Fe}^{\text{III}}(\text{L}^5)(\text{NCSe})]$. This complex exhibits a thermally induced spin crossover centered at $T_{1/2} = 270$ K with no thermally induced hysteresis. The X-ray structure analysis confirms a presence of two independent units: at $T = 293$ K both are high-spin but at $T = 100$ K one is low-spin ($S = 1/2$) and the second is frozen in the high-spin state ($S = 5/2$). This assignment is also confirmed by the Mössbauer spectra and matched the fitting of the magnetic susceptibility data.

Keywords: Fe(III) complex, spin crossover, Schiff base

Morphological response of amaranth plants (*Amaranthus* spp.) to selected toxic metals

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Abstract: Neglected or minor species like amaranth (*Amaranthus* spp.) can markedly contribute to promoting environmental sustainability, agrobiodiversity enhancement and global food production. There is evidence that amaranth has the ability to tolerate and accumulate high concentrations of heavy metals from soil. Several studies have investigated growth responses, metal transportability and accumulation and phytoremoval capability in *Amaranthus* spp. However, little is known about the molecular mechanisms involved in the defense strategy against abiotic stress.

In the present study, we investigated the morphological response and phytoextraction capacity of grain amaranth 'Pribina' (*A. cruentus* L.), 'Zobor' (*A. hypochondriacus* x *A. hybridus*) and commercially preferred variety Plainsman (*A. hypochondriacus* x *A. hybridus*) exposed to two toxic metals – cadmium (Cd) and lead (Pb). Our results showed that the tested varieties could tolerate applied metal ions without lethal effects, but growth was reduced. Pb treatment was notably manifested by significantly reduced root surface area. The varieties were capable of absorbing a high level of Cd and Pb, predominantly in the roots, with limited root-to-shoot translocation. Thus, tested varieties can be used as potential phytostabilizers of Cd and Pb. Moreover, the most tolerant variety to these toxic metals was 'Pribina' (*A. cruentus* L.).

Keywords: amaranth, heavy metal accumulation, root to shoot translocation, morphology

Biochar- and PGR-assisted phytoremediation of complex contaminated sediments with *Paulownia tomentosa*

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Abstract: Phytoremediation optimisation is crucial for the sustainable remediation of complex contaminated sites. *Paulownia tomentosa* is a promising candidate due to consistent biomass production and the ability to accumulate trace elements and organochlorine pesticides.

Sediments from Hajek, CR (GPS 50°17'31.5" N 12°53'35.2" E), showed contamination exceeding MPC by up to 64.7 times for certain elements and 10 times higher for HCH isomers. To enhance phytoremediation, plant growth regulators Charkor and Stimpo, along with biochar from Agmeco LT., Brno, CR, were applied. The application rates of Charkor, Stimpo, and biochar were 0.25, 0.50, and 5%, respectively.

PGRs significantly reduced biomass metrics possibly due to increased root cell membrane permeability, leading to higher contaminant uptake alongside nutrients, while biochar increased. Charkor and Stimpo decreased plant height, stem diameter, leaves and stem DW by 30.4 and 28.9, 33.3 and 54.8, 61.8 and 77.1, 72.2 and 82.4%, respectively. However, when biochar was added along with PGRs, their negative effects were nullified or even surpassed the control. Solely applied biochar improved most parameters measured (except stem diameter and leaves quantity) by up to 196%, likely due to increased plant tolerance.

Study findings substantially contribute to novel strategies for treating emerging contaminants and achieving zero pollution.

Keywords: *Paulownia tomentosa*; HCH; sediments; biochar; phytoremediation

Slow magnetic relaxation in mononuclear Mn(II) complexes

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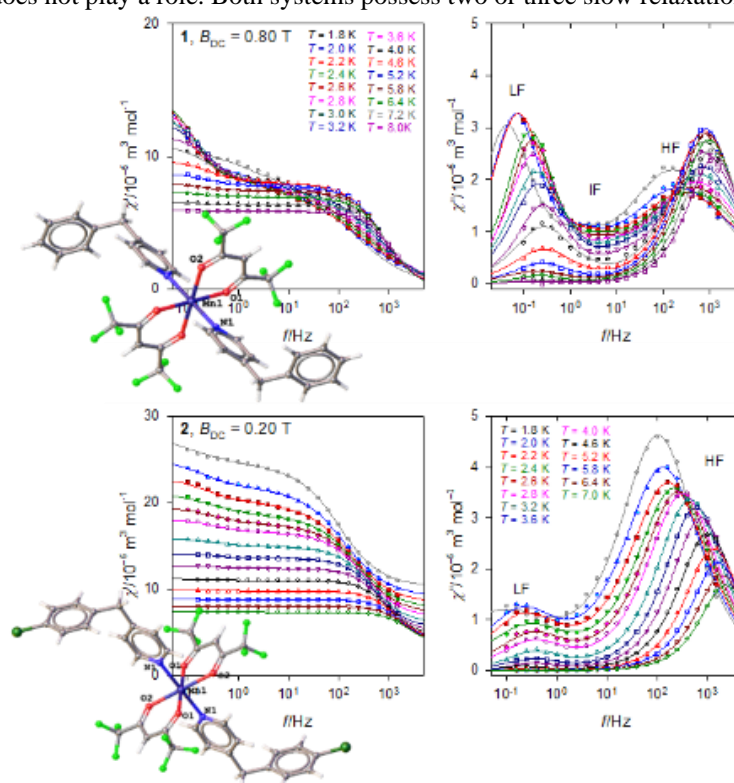
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Abstract: Two hexacoordinate Mn(II) complexes containing a chelating residue of hexafluoroacetylacetone and (Cl-substituted) 4-benzylpyridine show DC magnetic functions typical for $S = 5/2$ spin systems: $g \sim 2$, D – small. The AC susceptibility confirms a field supported slow magnetic relaxation in which the over-barrier Orbach relaxation process does not play a role. Both systems possess two or three slow relaxation channels.



Keywords: EPR, Mn(II) complexes, slow magnetic relaxation

Acknowledgement: Slovak grant agencies (APVV 18-0016, APVV 19-0087, VEGA 1/0191/22, VEGA 1/0078/21 and VEGA 1/0086/21) are acknowledged for their financial support.

Impact of soil amendments on the production of *Miscanthus × giganteus* biomass at the slightly contaminated post-mining areas

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Abstract: The physiological properties of *Miscanthus × giganteus* ($M \times g$), a second-generation energy crop, allows it to adapt to different soil conditions. The plant has a relatively high biomass yield and cellulose content, which makes it a promising feedstock for the production of biofuels and bioproducts.

The aim of this research was to monitor the bio-parameters, and study the change in the soil nematode communities during vegetation of $M \times g$ in the post-mining soil treated by various amendments in Chomutov, Czech Republic. Two fields; Field established in 2020 (F2020) was supplemented with NPK, biochar + NPK (BNPK), digestate (D), and sewage sludge (SS), and field established in 2021 (F2021) was supplemented with two doses of biochar; 5 and 10% (BD1 and BD2), D, SS, and hemicellulosic waste (HW). The bio-parameters of $M \times g$ were assessed during three growing seasons for F2020 and two growing seasons for F2021.

Results showed that for F2020, D had a positive impact on the number and DW of $M \times g$ plants. For F2021, BD1, BD2 and D had positive effects on $M \times g$ development. During the first vegetation, the nematode communities were assessed for F2021 where SS and D favored a more stable maturity status of the nematode community.

Keywords: energy crop, soil amendments, biochar, biomass productivity

Green roof substrate amendment with sewage sludge biochar and its effect on chemical leaching: a field study

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Abstract: The treatment of sewage sludge (SS) is becoming a serious issue in the wastewater treatment cycle in European Union. One of the promising strategies is pyrolytic transformation of nutrient rich sewage sludge to carbonized product – biochar for environmental applications. In this work, SS biochar was applied as innovative additive to extensive green roof substrate at application rate 0, 10 and 20% (v/v) and its long-term impact on runoff quality was monitored on experimental green roof established in October 2020 on a rooftop of the Faculty of Education of the University of Trnava. Platforms with substrate mixtures (SB0, SB10, and SB20) were planted with Sedum plug plants and besides routine analysis of pH, EC, TSS, and COD in the runoff, water quality concentrations were used to monitor nutrients (TN, TP) and metals (Cd, Cu, Fe, Mn, Pb, and Zn) leaching. Our results show that the application of SS biochar did not significantly affect pH, EC, TSS and COD of runoff water. Higher EC and COD values in runoff from SB10 and SB20 compared to SB0 were observed only after the first precipitation events while fluctuating of pH and TSS values appears to be related to erosion and substrate degradation during the winter period. Both TN and TP concentrations in runoff were significantly higher after the first leaching, compared to the subsequent progression, suggesting that the substrates display first-flush behaviour. Overall, both TP and TN concentrations have decreased in runoff over 30 months of study and the addition of SS biochar at 10 and 20% application rates did not pose a greater risk of water contamination than the conventional extensive substrate. Although application of pyrolyzed sewage sludge led to an increase in the concentrations of some metals (Cu, Pb and Zn) in SB10 and SB20 substrates, no significant differences in metal leaching were found between the substrates and runoff did not exceed the maximum metal concentrations for irrigation water according to US EPA and FAO guidelines. This confirms that pyrolysis process transforms mobile forms of metals in sewage sludge into stable and relatively stable forms, and thereby significantly reducing their mobility. Based on our results, we suppose that sewage sludge-based biochar could be used as a valuable and water safe component of extensive substrates for green roofs.

Keywords: extensive roof substrate, sewage sludge biochar, runoff water quality

Acknowledgement: This research was funded by the Slovak Research and Development Agency under the contract number SK-AT-20-0004.

***In silico* analysis of the α -amylase family GH57 to identify new groups of putative proteins with incomplete catalytic machinery**

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Abstract: Currently, the CAZy database classifies 183 families of glycoside hydrolases (GHs). Four of them – GH13, GH57, GH119 and GH126 – can be considered the α -amylase families. This *in silico* study has been focused on the family GH57. Its members employ the retaining reaction mechanism, dispose five conserved sequence regions (CSRs) and possess an incomplete TIM-barrel with a succeeding α -helical bundle. The GH57 catalytic machinery consists of catalytic nucleophile (Glu at the strand β 4 in CSR-3) and proton donor (Asp at the strand β 7 in CSR-4). The detailed sequence comparison of the entire family – i.e. 4,591 sequences (actual in March 2023) has been performed in an effort to find out potentially new groups of GH57 members with complete or incomplete catalytic machinery. This goal was achieved by creating the evolutionary trees focused on the enzyme specificities and enzyme-like homologues recognised in the family previously. The trees were based on both the intact complete sequences and also on five well-established CSRs. In addition to refining the sequence details in sequence logos characteristic of individual enzyme specificities, the recent increase of GH57 sequences allowed to identify a new group of proteins with incomplete catalytic machinery related to amylopullulanases, the so-called APU-like homologues.

Keywords: α -amylase family GH57, enzyme specificity, conserved sequence regions, evolutionary relatedness, protein homologues

A detailed *in silico* analysis of the α -amylase family GH126 focused on its unique sequence-structural features

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Abstract: The creation of the CAZy family GH126 was based on a partial biochemical characterization and tertiary structure determination of the amylolytic enzyme CPF_2247 from *Clostridium perfringens* as a potential α -amylase family. Taxonomically, it contains proteins of bacterial origin only. The members should adopt the catalytic (α/α)₆-barrel domain, but neither catalytic machinery, nor the reaction mechanism has been determined as yet. This insufficient characterization together with sequence-structural similarity of GH126 members to those of the clan GH-M (families GH8 and GH48) may lead, however, to incorrect classification of putative proteins. Therefore, the main goal of the present study was the identification of unique sequence-structural features that would definitively distinguish the family GH126 from both GH8 and GH48. For this purpose, a sequence logo representing the seven conserved regions specific for the family GH126 was created using 1,475 GH126 sequences, along with 86 and 75 sequences from family GH8 and GH48, respectively. Although the putative GH126 catalytic and/or active-site residues have been found most probably shared with the clan GH-M, a detailed comparison of 50 selected representatives, supported by BLAST searches, allowed for defining the sequence positions that should be unique for each of the three families.

Keywords: α -amylase family GH126; catalytic (α/α)₆-barrel; *in silico* analysis; unique sequence-structural features; conserved sequence regions; evolutionary relationships

The occurrence of *Vibrio cholerae* non-O1/non-O139 in rivers of Slovakia

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Abstract: Bacteria of the genus *Vibrio* are found in aquatic habitats worldwide. Strains of *V. cholerae* non-O1/non-O139 can cause diarrheal diseases and extraintestinal infections in humans, including ear infections, wounds infections and septicemia. Infection can occur after recreational activities such as swimming, rafting or fishing. Due to global warming, the number of infections caused by vibrios is increasing worldwide, making these bacteria emergent pathogens. We focused on the occurrence of *V. cholerae* non-O1/non-O139 in selected aquatic habitats of Slovakia. We collected water samples three times, during summer, autumn and winter, from the rivers Topľa, Ondava, Danube and Morava. We isolated and identified strains of *V. cholerae* non-O1/non-O139 in the Danube, Topľa and Ondava rivers, but not during all samplings and not in river Morava. When growth conditions are not optimal, vibrios can enter a physiological state, when they are viable but non-culturable (VBNC). Interesting is the possible clonal diversity within one watercourse indicated by the diversity in the biochemical tests of the ENTEROtest 24 system (Erba Lachema, Czech Republic) of isolates originating from one water source. Detailed molecular characterization of isolates is planned.

Keywords: *Vibrio cholerae* non-O1/non-O139, *Vibrio* spp., aquatic habitats of Slovakia, emerging pathogens



Acknowledgement to Sponsors





ANS 2023

The 8th International Scientific Conference
Applied Natural Sciences 2023

Book of abstracts

Editor
Martin Valica

Title: Applied Natural Sciences 2023 – Book of Abstracts
Publisher: University of Ss. Cyril and Methodius in Trnava (Slovak Republic)
Edition: 1st, 2023
Pages: 94



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ISBN 978-80-572-0357-5